Aspen Plus Simulation Software – A Basic Course for Beginners

Prof. Prabirkumar Saha
Department of Chemical Engineering
Indian Institute of Technology, Guwahati

Lecture - 31
Hydrodealkylation of Toulene

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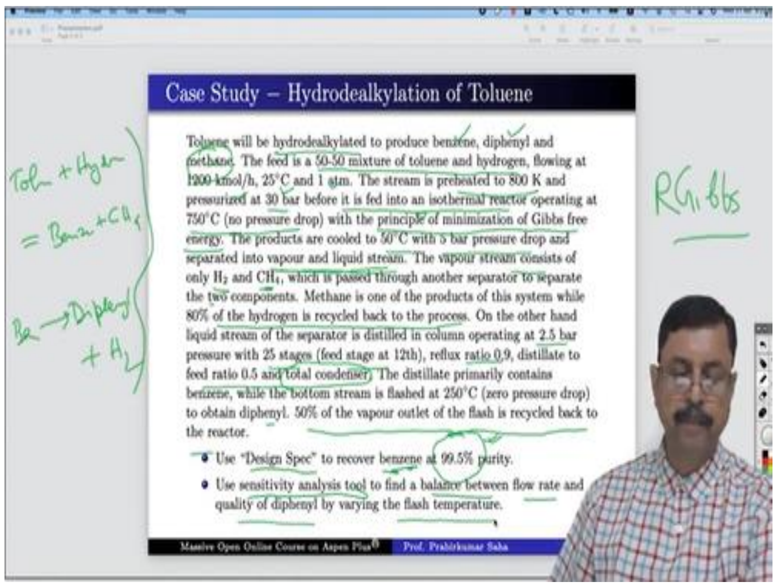

Welcome to the massive open online course on Aspen plus. Today, we shall perform yet another interesting case study and that is on hydrodealkylation of toluene. Now, as we understand toluene has a structure of this nature, where there will be a CH_3 attached in the benzene ring. So, we will de-alkylate this that means, this CH_3 bond will be removed and we shall produce benzene and methane and then benzene will subsequently produce diphenyl.

So, we have toluene plus hydrogen that will produce benzene and methane. And, later benzene will produce diphenyl plus hydrogen. So, this is a complete reaction mechanism. So, the entire process we shall perform through Aspen plus simulation. Now, the problem statement is something like this, toluene will be hydro de-alkylated to produce benzene diphenyl and methane.

Now, this feed is having 50-50 mixture of toluene and hydrogen, whose flow rate temperature and pressure has been given, the stream is preheated to 800 kelvins and has been pressurized to 30 bar before it is fed into the isothermal reactor operating at 750 °C. The reactor will run with the principle of minimization of Gibbs free energy. So, basically, we will use an R Gibbs block of Aspen plus simulation.

The products are then cooled to 50 °C with 5 bar of pressure drop and it will be separated into vapour and liquid stream.

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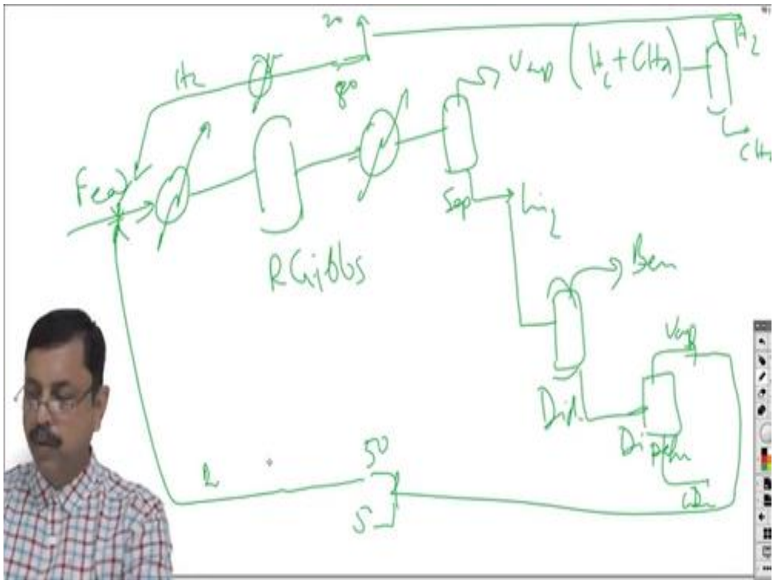

So, we shall have a feed which will be pre-heated then it will go through and R Gibbs block of Aspen plus then it will be cooled again and then, it will pass through a separator. The separator will separate them into vapour and liquid stream. So, they will have vapour and liquid stream, and then the vapour stream consists of only hydrogen and CH_4 So, we will have here hydrogen and CH_4 over here which is passed through another separator to separate these two components.

So, we will have another separator which will separate them into H_2 and CH_4. Then, methane is one of the products of this system, that we know methane is one of the products whereas 80% of the hydrogen is recycled back to the process. That means we will have this hydrogen over here, so we will split them into 20 and 80% and that 80% will come back to the feed stream as a recycle. Obviously, we have to do this pressure and temperature correction over here.

On the other hand, liquid stream of the separator is distilled in a column. So, we will have this, we will have a distillation column over here. In that distillation column, we have the pressure, number of stages, feed stage, reflux ratio and distillate to feed ratio have been given and it is also said that it will have a total condenser. So, this liquid stream will be passed through the distillation column and this distillate will primarily contain benzene.

And bottom stream will have diphenyl. So, we have the distillate, we will have benzene over here and here we will have diphenyl. And then the bottom stream is flashed, so this bottom stream will be flashed obviously here we will have a vapour phase, here we will have a liquid phase. This liquid phase will contain mainly the diphenyl. We do not know what will be there in the vapour phase.

But it is said 50% of the vapour phase outlet of the flash will be recycled back to the reactor. That means, this will be again pass through a splitter 50-50 and this 50% will be fed back to the feed line. So, feed line will have two streams as recycle and one stream will have pure hydrogen and another stream it will also have some diphenyl and maybe some portion of benzene or we do not know what we will have.

But definitely it will have something of interest. We will understand it later, while we solve the problem. Now, these are the tasks that we have to do. We have to use design spec to recover benzene at 99.5% purity. So, to attain this purity if we have to lose some portion of benzene that we have to accept. And, also, we have to do some sensitivity analysis to find a balance between flow rate and quality of diphenyl by varying the flash temperature.

So, in the problem statement it has not been said, what is the quality or what is the flow rate of diphenyl that we desire. Obviously, if you increase the quality of diphenyl the quantity will decrease. If you increase the flow rate of diphenyl, the quality will decrease. So, we have to have a balance between quality and quantity. So, that decision we have to take by analysing it through sensitivity analysis. So, let us solve the problem in Aspen plus window.

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So, here let us have hydrogen, methane and finally diphenyl. So, we have to choose a method name in the problem statement they have not given any or they have not suggested any method. But we have done so many case studies and we understand that in this kind of situation when you have benzene, we have toluene always we have done with Peng-Robinson property method. So, here also we shall choose Peng-Robinson property method.

So, let us choose Peng-Robinson over here and run the property analysis. Once it is done, we have to go to the simulation window; yes, it is done, so let us go to the simulation window and, first let us do only this portion. So, we have the feed, the preheater and the R Gibbs reactor. So, for that let us choose a heater model and one R Gibbs model over here. So, we have R Gibbs model and heater, we have to attach the feed line, this is the connection and this is.

Now, if you look at this you will have one mixer over here. So, let us not forget the mixer. So, let us choose this one and then we will reconnect the destination at this point and we will have the material stream which will come out from here and it will be attached to this end. Now, we have two more ends which will leave for the recycle feeds. Now, we have to rename them, so rename it as feed and this is the mixer. So, mixer one or we all have only one mixer.

So, let us say mix and this is the feed plus recycle stream and obviously it will be a preheater so let us try preheat and this is the reactor in, this is reactor out and this is obviously the reactor. So, that we will keep it over here, now press next it will definitely ask for the components in feed.

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So, let us see the problem statement, we will have the feed is 50-50 mixture of toluene and hydrogen flowing at 1200 kmol/hr. That means, there will be 600 kmol/hr of toluene, 600 hydrogens and there will be 25 °C one atmosphere pressure.

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So, we will have 25 °C one atmosphere pressure, so we will keep it atmosphere over here and then 600 toluene and 600 hydrogen or else you could have given 1200 over here and write 0.5 0.5 as mole fractions of toluene and hydrogen, whatever way you want you can give. Then, press next it will ask for the preheater condition.

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So, let us go back to the problem statement, we find the stream is preheated to 800 kelvins and 30 bar pressure.

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So, we will have 800 kelvin and 30 bar pressure. So, press next, it will ask for the condition of RGibbs, the reactor operating at 750 ℃ and no pressure drop. So, 750 ℃ and no pressure drop. So, everything is fixed, so it will calculate the phase equilibrium and chemical equilibrium as well. So, run the simulation so we have got the result. So, go to the reactor stream results and you will find.

Here you will find 202 kmol/hr of benzene has been produced, toluene has reduced from 600 to 38 hydrogen had reduced from 600 to 37 so they remain unreacted. We have 675 kmol/hr of methane and 170 kmol/hr of diphenyl. Now, these figures will improve once we do the recycling. Now, first let us freeze this screen, this screen say screen number 1.

This lets you know what will be the product of the reactor without any recycle, it will be without any recycle. Now, we shall do the first recycle and check what are the betterment that we get. So, for that let us go back to the simulation. First, we have to cool down and then we have to keep two separators in series. In this separator we have to separate hydrogen and methane and then this hydrogen and methane will be separated over here. So, first let us do this portion.

So, for that let us add one separator over here, so this is the first separator. It will separate hydrogen and methane from others and then we will have another separator that will separate hydrogen and methane. And we will have these connections from here to here, then we will have this one and we will have this one and we shall connect these two and then this will have another outlet. So, we will have this as separator 1 this is separator 2.

So, we will keep it on the icon, so that it does not clutter. And this one we write SEP1 vapour, this one is SEP1 liquid, this one is SEP1 or SEP2 vapour, and this one is SEP2 liquid. Now, this condition sep1 will separate hydrogen and so, vapour of separator one will contain only hydrogen and methane all others will be 0. So, this is done and sep2 will have only hydrogen in the vapour phase, there will be no methane.

And other things anyway they will be 0, even if you do not write it will take 0 itself. So, let us run the simulation and check what we have. Now, if we take the temperature, pressure and more flow rate, you will find over here the temperature and pressure, they are 750 ℃ 30 bar pressure. Well, we have missed something, what we miss? We should have given a cooler over here, and that we have missed.

So, let us go back and put a cooler, otherwise the separator will not work as per expectation. It is giving some value, output value but the liquid phase of separator that will not function, when we will use a distillation column. So, what we have to do? We have to put an exchanger over here, so let us put an exchanger and this outlet has to reconnect to the cooler and this will have a material stream that will have a connection with the separator.

So, here we rename it as a COOLER and this one will write sep1 in and then the cooler condition we have to say, what is that? The products are cooled to 50 ℃ with 5 bar pressure drop. So, we will have 50 ℃ outlet of the cooler and there will be a pressure drop of 5 bar, so we write - 5 over there. And then, we run the simulation once again and we have got the result quickly.

And here we find that temperature and pressures are 50 ℃ and 25 bar and there will be a mole flow rate of 38. So, let us go to separator 2 and check, what are the outputs stream results. Separator 2 vapour phase it will only have hydrogen. So, it will be 37.7198 kmol/hr of hydrogen will be there in the vapour phase, whereas 675.417 kmol/hr of methane will be produced and it will be separated.

Here we know that, methane is one of the products of the stream while 80% of the hydrogen is recycled back to the process. So, this is our product number 1, this methane and this vapour which is completely hydrogen, we will have 80 20, so it is 20% is parched and 80% has to come over here and mixed. But, one thing is there that, its temperature and pressure they do not match with them.

So, we have to cool down from 50 ℃ to 25 ℃ and there will be a pressure drop of 25 bar to 1 atmosphere pressure. So, we will have a cooler along with a pressure drop of 24 bar. So, let us add these two things. So, we shall have one splitter and that splitter will split 80, 20 and we will have one exchanger also. And then this one will have a rotate icon flip horizontal this also will flip horizontal.

So, that when we want to connect it; it gives a direction leftwards and we shall have these two connections, we will have these two connections. And there will be another material out that will be from here to here. So, this is the purge, so we will have H_2 purge, this is SPLITTER 1, this is 80% recycle and this is recycle1. We will have a second recycle, so we write it RECYCLE 1 and this one this is another cooler.

So, COOL 2 put it on the icon. So, now let us press next, so COOL 2 obviously the temperature will be 25 ℃ and pressure will be 1 atmosphere, so that it does not have any problem in mixing with the feed. And then, what next, yes splitter. So, H_2 purge will have 20% output, so 0.2 of hydrogen flow. So, H_2 will have 0.2, H_2 purge will have 0.2 and rest will go the 80% will go through COOL 2. So, now it is ready to run, so run it.

Now, go to this one SEP2 and see the stream results. Here check, what is the amount of methane? We have 693 kmol/hr, let us check this one, this result is with RECYCLE 1. We have connected only one recycle loop. So, it is with RECYCLE 1 and we have got 693.793 kmol/hr. Compare it with the previous one, so this is without any recycle. How much did you get? It is 675.417. So, here it is 675 and here it is 693.

So, obviously we have increased the production of methane with a recycle stream. So, one recycle stream is complete. Now the second one we have to see, what is there in SEP1 liquid. So, these portions we have never seen just go to stream result of SEP1 and check what is there in SEP1 liquid. You will find we will have 203 kmol/hr of benzene, 167 kmol/hr diphenyl and 38.9 so maybe 39 kmol/hr of toluene, unreacted toluene.

So, here we have to recycle the toluene part. So, this toluene has to be recycled, benzene and diphenyl they are our products. So, first let us use the distillation column over here, so we will use distil over here, connect this thing and then this is the material stream. And this one is let us write dist and this one let us write bottom. The liquid stream of separator is distilled in a column all this information will be needed for us.

We have 25 stages, 12th feed stage recycles ratio 0.9 distillate to feed ratio 0.5 and total condenser will be used for distillation column. So, we will have, so it is 25, 12 is the feed stage, reflux ratio 0.9, distillate to feed mole ratio 0.5, total condenser and condenser re-boiler pressure, it was operating at 2.5 bar. So, we have 2.5 bar, done. So, let us rename this as DISTIL, so distillation column and then if we run it.

Now, let us check the output of distillation column and see the stream results. And you will find over here, we have 203.018 kmol/hr of benzene and 1.98 toluene. In the bottom we have most of the toluene and diphenyl, very small amount of benzene. In terms of mole fraction, it is already 99% benzene in the distillate which obviously we have to take to 99.5%. And here diphenyl percentage is 81.89 which we have the scope to improve.

And toluene percentage is 18% and this toluene has to be recycled. So, the distillate primarily contains benzene obviously this is true, while the bottom stream is flashed at 250 ℃ with 0 pressure drop to obtain diphenyl and the 50% of vapour outlet of the flash is recycled back to the reactor. So, we already have 99% of benzene over here and bottom is having 81% of diphenyl and 19% of toluene.

So, this has to be passed through a flash and obviously this flash will contain mostly toluene, the vapour phase and liquid phase will be diphenyl. Let us see whether it happens so. Let us attach a flash and attach this one take a material out and this one out. Now, we have to rename them, rename it as FLASH. This is FLASH liquid and this is flash vapour and flash will operate at 250 ℃ with 0 pressure drops.

So, flash will operate at 250 ℃ with 0 pressure drop. Now, let us run it and check the stream results of flash and as expected we have 88% of diphenyl is going through the liquid and here, we have 11% to 12% toluene as well. But in vapour phase almost there is no diphenyl, no benzene only toluene. So, vapour phase will have toluene 15.29 kmol/hr of toluene and 21 kmol/hr of toluene will go through the liquid phase of flash.

So, basically this liquid phase is the product and vapour phase that is with toluene has to be recycled not everything 50% will be recycled and 50% will be purged. At least that is what has been written in the problem statement. If you see, 50% of the vapour outlet of the flash is recycled back to the reactor. So, what we will need to do? We have to add a recycle. But before that, let us see the design spec to recover benzene at 99.5% purity.

Now it is 99% purity for benzene, we have to go to 99.5% and we will use design spec for that. So, let us use the design spec, it is there in the manipulator. So, we have the design spec over here, so use this icon, it is a very good icon. Just put it over here, rename it as DESIGN SPEC and then double click to give the parameters. Now here we have to write the new thing which is BENQUA that is the quality of benzene.

And what is it? It is basically mole fraction of stream, distillate and the component benzene. And what will be the spec of BENQUA? It should have a target of 995 and we will give a tolerance limit of 0.0001 and we will vary the distillate to feed ratio which is 0.5, so we shall vary this. We will vary the block variable of block distil; the variable is D2F. Let us have a lower limit of 0 and upper limit of one, let us check within that limit.

Right now, it is at 0.5 and we do not know where it will reach. So, let us run it, it has run very fast, go to the result and we will find the final value at 0.497. So, it is very near actually 0.497289. At that point, we will have 0.9949; we have given 0.0001 tolerances, so we have to accept it. So, it is 0.497289, so we copy this number and instead of 0.5 we write 0.497289. And go back to your design spec and just deactivate because we do not need the design spec now.

Because we; have arrived at the desired D 2 F ratio. So, now if we run once again, you will find 99.5% purity in distillate. So, just cross check, do not have to believe me, just go to the stream result and go to the distillate rate, mole fraction you will find 0.994934 for benzene. So, it is 99.5% purity. Now, the second task which is use sensitivity analysis tool to find a balance between flow rate and the quality of diphenyl by varying the flash temperature.

Now, we can do the sensitivity analysis after we recycle or before we recycle. Now, let us do it both after and before and see what difference we will have. So, before recycling if we do, then we have to do this sensitivity analysis over here in model analysis tool, go to sensitivity check new. So, what will be very? We will vary flash temperature and so we will vary block variable which block flash, which variable it will be temperature.

Now, at this moment the flash works at temperature 250 ℃, so we will give between 240 and 260 or 230 and 270. So, let us give between 230 and 270. So, 20 up and 20 down and let us check what happens. And we will have an increment of say 1 ℃, so it will have 230, 231, 232, 233 etcetera and then we have to define. So, we will define two things, one is diphenyl fluoride and diphenyl quality.

So, first one; diphenyl chloride and diphenyl quality; these two things, so, first let us define flow rate which is a mole flow type. So, this is mole flow of stream, it should be flash liquid. So, flash liquid and component diphenyl and diphenyl quality again it will be a mole fraction this time of the stream, flash liquid of the component diphenyl again. So, both the flow rate and quality of diphenyl has been defined and will tabulate both of them and then run it.

So, running will it has taken no time and generated the results, so we have got the result from 230 ℃ to 270 ℃ and we see as the temperature increases, we have less and less flow rate of diphenyl and betterment of quality of diphenyl. So, fluoride gets reduced with temperature while quality increases, and this is expected. So, let us plot it and see how it looks.

So, for x axis we will put the temperature and in y axis we will put diphenyl flow rate and diphenyl quality and press ok, we will get a plot. Now, let us check. The decision is up to us. So, we will find over here as the temperature increases the quality increases, but quality also it does not go beyond 93.5%. Obviously, if we connect the recycle stream, we can expect this quality to increase.

But without the recycle we can never go beyond this, unless if we increase the temperature obviously, we can go beyond 93.5. But even with 93.5 the flow rate decreases to 134, so from 168 to 134 it reduces by 30 kmol/hr. So, it is up to you to decide, where exactly will cut the line. So, if you see that I cannot compromise with my quality then you have to be content with this much of quantity.

But, if you say that I can manage with even 80% or 87% of quality, then obviously you will have much higher flow rate of diphenyl. So, this decision you have to take and this will be dependent upon the requirement at the customer's end. And, for the time being let us deactivate the sensitivity analysis and we will recycle the stream. So, for recycling this FVAP we have to first split.

So, we will have a split over here and this split first we will rotate the icon and flip vertically also. And then, we will connect this thing in this fashion, so this is our product and this is recycled and then this will go to the recycle stream and one more will come from this end and we will say this is our purge. So, this will rename as RECYCLE 2, this is SPLIT 2, again we have done a mistake over here.

We have to have a mistake over here, because here the temperature is 250 ℃ and pressure is 3 bar or if we check the FVAP 250 ℃ and 3 bar so it should be 25 ℃ and one atmosphere. So, again we have to have a heater or let us say cooler and that cooler has to be rotated icon. And this one should be reconnected to a different source, which is this one and this outlet has to connect to it this one.

So, you have this one as cool 3 because this is the cooler 3. This one is cool 3 in this one is purge 2. So, this is H_2 purge, we can say deep purge also or toluene purge also, no problem, and all other things are renamed already. So, now we have to specify the cool 2 which should be 25 ℃ and 1 atmosphere. So, 25 ℃ and 1 atmosphere. So, that it does not have any problem in mixing with the original feed stream.

And now, let us recycle. Split to obviously it is 50-50. Let us go back to preview, 50% of vapour outlet and of the flash is recycled back. So, it is 0.5 and now you can run. So, press run, so it is over. Now again you check the liquid flash. What is the output stream result? You can see the molar flow rate of F liquid is 165.628. The total molar flow rate is 173, obviously with RECYCLE 2 it has increased, so if we say this is with RECYCLE 2.

And now, compare it without recycle; we have to compare this bottom product 173 diphenyl and toluene 37.64. So, go back to without recycle, this is without any recycle. You can check the diphenyl content 170 whereas; right now, we are getting 173. So, clearly there is an increase in diphenyl. Now, the obviously the increase is only 3 kmol/hr but with recycle it has increased, that much we can guarantee.

Now, one problem is left we have to do the sensitivity analysis once again with the recycle stream connected. So, we go back to the sensitivity analysis and press active and do the run once again. So, now they are producing some error in the result and we have to check with 230 probably it is not having any good results. So, 230 maybe a 2 lesser temperature; for flash when a recycle loop is there.

And is there any problem with the higher rate? There is no problem in the higher rate. We can go even higher at 93.365. So, let us check the plot once again. So, this is the plot that we are getting now, it is meeting somewhere at 256 ℃, here it was near 254. So, with more and more refined simulation, we can shift the point of intersection towards this side. That means both the quality and the flow rate, both will be better if our simulation is refined further or our process is refined further.

So, that is the conclusion that we can arrive at. So, we have done both these tasks and we have completed the simulation as it is stated.

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So, with that we conclude our case study on hydrodealkylation of toluene. And in the next lecture we will come up with another interesting case study. Till then thank you and goodbye.