Aspen Plus Simulation Software – A Basic Course For Beginners

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Lecture-25

Introduction to the Course and Basic principles of Image Formation

Welcome to the massive open online course on aspen plus.

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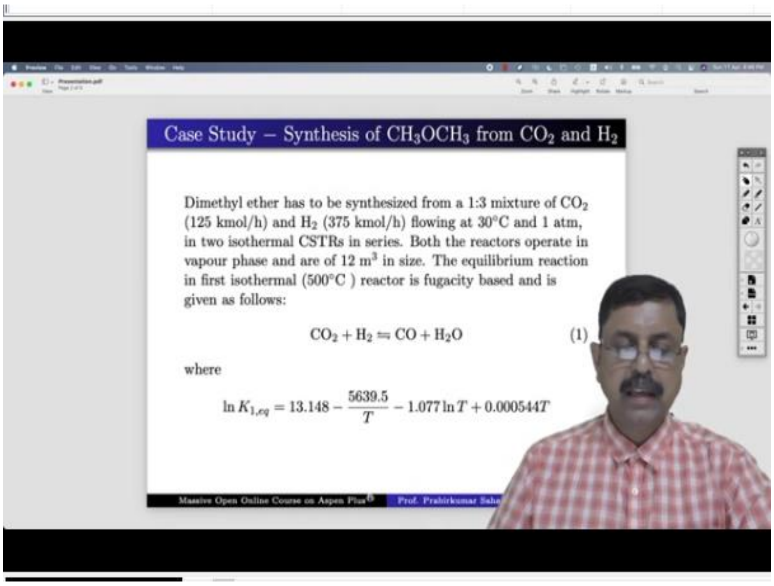

In today's lecture, we shall perform another case study about dimethyl ether synthesis from carbon dioxide and hydrogen. So, dimethyl ether has to be synthesized from a 1 is to 3 mixture of CO_2 and H_2 as we understand that the flow rate of carbon dioxide is 125 kmol/hr and that of hydrogen is three times that is 375 kmol/hr, and they are flowing at 30 ℃ and 1 atm pressure.

And this synthesis has to be done in 2 isothermal CSTRs in series, and both these reactors operate at the vapour phase, and their size is given, which is 12 m^3 each that is 12000 liters for both the reactors. The equilibrium reaction in the first isothermal reactor is 500 ℃, and it is fugacity based the reaction is given below where this particular equation provides the equilibrium with K_1.

$$CO_2 + H_2 \leftrightharpoons CO + H_2O$$

$$lnK_1, eq = 13.148 - \frac{5639.5}{T} - 1.077lnT + 0.000544T$$

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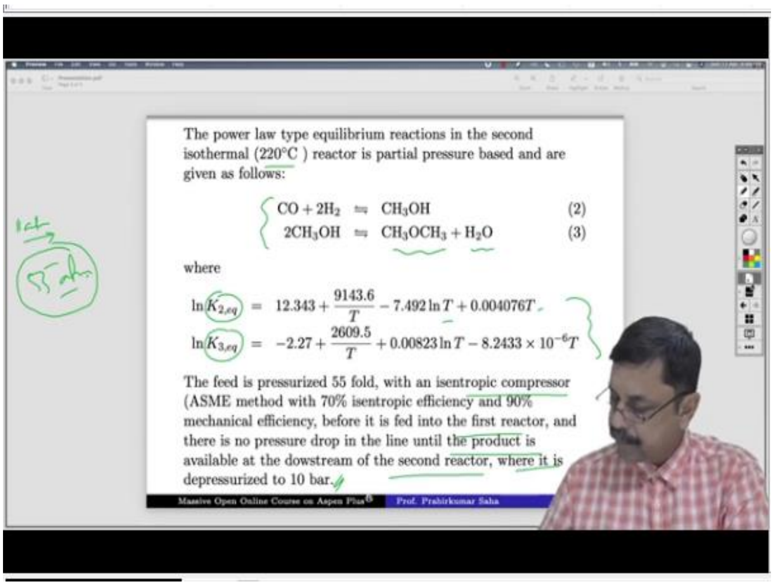

To continue with the second reactor, which is power law type equilibrium reaction and the temperature of the second reactor is 220 ℃ and it is partial pressure based and there are 2 reactions; in the first carbon monoxide reacts with hydrogen to form methanol and then methanol gets dissociated in dimethyl ether and water. And the equilibrium parameter for both of them as a function of temperature is given in these two reactions.

$$CO_2 + 2H_2 \leftrightharpoons CH_3OH$$

$$2CH_3OH \leftrightharpoons CH_3OCH_3 + H_2O$$

$$lnK_2, eq = 12.343 + \frac{9143.6}{T} - 7.492lnT + 0.004076T$$

$$lnK_3, eq = -2.27 + \frac{2609.5}{T} + 0.00823lnT - 8.2433 \times 10^{-6}$$

Now the feed is pressurized 55 fold that means our feed pressure is 1 atm, so it is pressurized up to 55 atm using an isentropic compressor before it is fed into the first reactor. There is no pressure drop in the line until the product is available at downstream of the second reactor, where it is depressurized at 10 bar. That means as we have pressurized it up to 55 atm pressure so what will it do?

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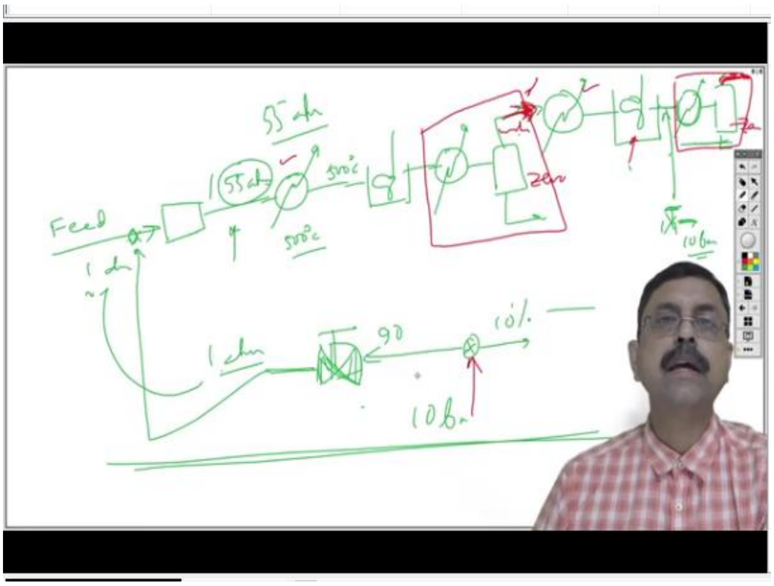

It will have a feed line with 1 atm pressure, we will use a compressor which will make it 55 atm and in the bargain we will increase the temperature a lot. Now obviously, this temperature will not be 500 °C which is the temperature of the first isothermal reactor. So, we have to use some heater or cooler for the temperature correction, and then here we will have 500 °C, and then we will have a reactor.

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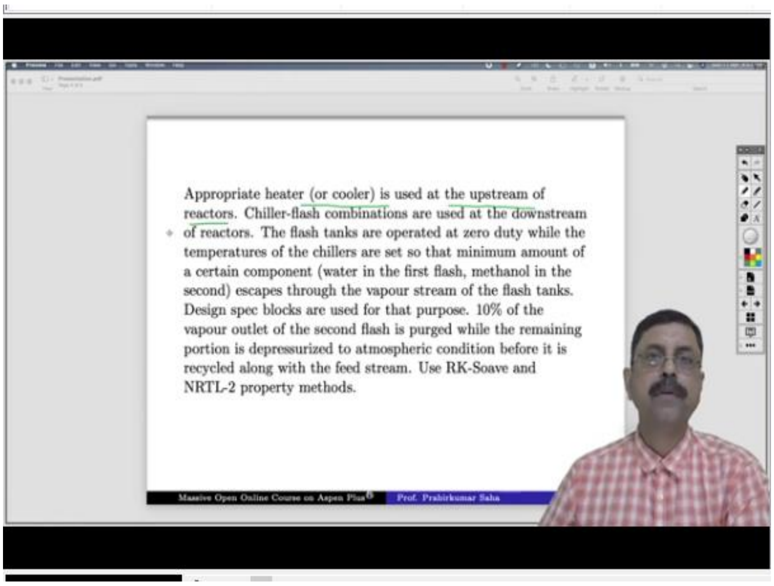

Now that is why it is written appropriate heater or cooler is used at upstream of the reactor. So, every reactor will have that heater or cooler before the feed is given into the reactor. Now Chiller-flash combinations are used at downstream of the reactor. So, the heater or cooler will not be only in upstream but also in downstream. So, each reactor will have one heater or cooler before and after the reaction is taken place.

And after that, we will have a flash. So, Chiller-flash combinations are used downstream of the reactor. So, basically, we will have a chiller over here then we will have a flash, and this flash outlet will go to the second reactor. In the second reactor, we will have another heater, and then we will have the second reactor, and after that, we will have another heater and a flash.

So, this is the Chiller-flash combination after the second reactor and this is the Chiller-flash combination after the first reactor and these 2 heaters or coolers will be at the upstream of the reactor. So, that is what we have over here. So, heater or cooler at the upstream, Chiller-flash combination at the downstream, and we also have this information. The flash tanks are operated at zero duty. At the same time, the temperatures of the Chillers are set so that the minimum amount of certain components that is water in the first flash and methanol in the second escapes through the vapour stream of the flash tank.

So, let us understand this, we have the flash tank, here we have zero duty but the vapour stream of these flash tanks, here we have to minimize something, this should be dry that means it should not have any water vapour and this will not have any methanol because this is either it will be recycled or some part of it will be purged. So, we want to minimize the methanol loss over here.

And here, also we want to minimize the water content at this point because the presence of water in this stream will affect the second reactor. So, these are the condition given over here. So, design spec blocks are used for that purpose. So, today we will learn how to use design spec. So, this is the new thing that we will learn today. 10% of the second flash's vapor outlet is purged while the remaining portion of the depressurized atmospheric condition before it is recycled along with the feed stream.

That means this one, this flash the vapour outlet of the flash will have 10% purged and 90% they will be first depressurized with a valve and that will be added in a mixer with the feed so, that it can be recycled. So, this is the total structure that we have, and one thing that we have missed here is that there is no pressure drop in the line until the product is available downstream of the second reactor.

That means between this reactor output and before feeding into the heater, we have to place one valve where it will be deep pressurized. So, from this point to this point, we had 55 atm pressure, and at the downstream, we had 10 bar pressure. So, from this line to this line up to this point, we will have 10 bar pressure, and after this, we will use a valve which will again bring it to 1 atm because unless we get it to 1 atm, we cannot add into the feed line.

This is the total structure that we will employ in the aspen plus window, and one more piece of information that we have over here that they have asked us to use RK-Soave and NRTL-2 property method. So, we shall use that. So, let us go to the aspen plus command window. **(Video Starts: 10:48)** So, we have to insert the component IDs, so the components are carbon monoxide, carbon dioxide, hydrogen and water.

And also we will have methanol and dimethyl ether that we have to find as dimethyl ether and we have to search for it, this is the one which we are looking for. So, let us change this name, it does not look good, DME seems good, so press next. So, we have to use RK-Soave, and then we have to use NRTL-2. So, these are the two property methods that we will be using.

So, just run once again until unless they become ticked, so the property method is set. Now let us go to the simulation window. So, let our run-up to the first reactor, so you remember this diagram, we have to use one compressor, one heater or cooler, and then one reactor. So, let us first use the compressor. So, this is the compressor, we have a heater, and we have a CSTR. So, write COM1 H1 and CSTR1.

Then attach the feed line, this line, this line, and this line, rename them as feed COM1 OUT then H1 OUT, and this is R OUT or R1 OUT. So, we have to give the information. Now for a change let us define the reactions now itself we refer to this and set the reactions. So, the first reaction is R1 which is the equilibrium type, we will have carbon dioxide and hydrogen -1, -1 which will form carbon monoxide and water.

There 1 and 1 and the equilibrium condition will be given by now this is vapour phase reaction and the temperature will be 500 ℃ because the reaction occurs at 500 ℃, compute k equilibrium the first reaction is fugacity based, this is fugacity based so write here fugacity and this is the same reaction a b by t c dt, so the same equation we have to write a, b, c, d like this.

$$lnK,eq = A + \frac{B}{T} + ClnT = DT$$

where. T in (K)

So, a is 13.148, b will be -5639.5, c is -1.077 and finally, d is 0.000544. So, this reaction has been defined, we press new, and the second reaction will be available with us. So, this is again an equilibrium based reaction, and the second reaction it is carbon monoxide plus 2 hydrogen, so carbon monoxide + 2 hydrogen will produce methanol. Only one and the second reaction, which is 2 methanol, produces dimethyl ether and water.

So, 2 methanol produces dimethyl ether and water. Now we have to set the equilibrium condition, it is vapour phase, and the second reactor it operates at 220 ℃. So, it is 220 ℃, compute the equilibrium this is partial pressure based. So, K equilibrium basis is partial pressure, a, b, c, d. So, the first reaction we have 12.343, 9143.6, - 7.492, and the last one is 0.004076.

And for the second reaction will be vapour phase and the temperature will be 2 to 0, partial pressure based -2.27 A, B is 2609.5, C is 0.00823, and finally, D is -8.2433×10^{-6}. So, reaction 1 and reaction 2 are set now we can go back to our main flow sheet. So, press next. Here the feed is given at a temperature of 30 ℃, 1 atm. So, 30 ℃ and 1 atm and the molar flow rate CO_2 125, H_2 375. So, this is 125 and 375.

So, 1 is to 3 ratio, total 500. Then press next again, it will ask for the compressor details, pressurized 55 fold with an isentropic compressor ASME method 70% isentropic efficiency and 90% mechanical efficiency. So, this is the ASME method, 55 fold means it will be 55 times the inlet. So, the pressure ratio will be 55, so it is not given discharge pressure; actually we can give 55 atm also, but here we have given pressure ratio.

Isentropic efficiency is at 70%, and the other one is at 90% mechanical efficiency. So, mechanical efficiency is 0.9, then it will ask for the reactor setup, and we can give 0 bar because there is no pressure drop in the line. You might remember that there is no pressure drop in the line until the product is available downstream of the second reactor. So, everywhere we will have 0 bar that means no pressure drop.

Temperature it will be 500 ℃ isothermal condition valid phases vapour only and reactor is 12 m^3 or 12000 liters the same thing, it is given over here you can recheck this 12 m^3 in size both the reactors, they operate in vapour phase and are of 12 m^3 in size. So, vapour phase, valid phase is vapour phase and volume is 12000 liters.

Reaction kinetics already we have defined just add it our job is done, press next, it will ask for the heater again the heater is set at 500 ℃, because we do not know how much temperature will be increased after the feed is compressed to 55 times it may be more it may be less. Still, we have set the outlet temperature of the heater as 500 ℃. So, no matter whether it is higher or lower, if the compressor outlet has a higher temperature than 500 ℃, this H1 block will act as a cooler; otherwise, it will act as a heater.

That we will learn later, and pressure obviously will put 0 because there is no pressure drop, and you can say valid phases as vapour only because there is no point in giving vapour liquid just give vapour only and it is ready to run. So, we have the information, let us check this information. So, the pressure is 1 atm before compressor 1 and after that it becomes 56 bar because it has multiplied 55 times.

Now as it is in bar and it is giving a whole number we can change the display option to one digit then it will show correctly, it is 55.7 not 56 actually it has increased 55 times and everywhere down the line it is 55.7 only, so there is no pressure drop in the line and the temperature increases from 30 ℃ to 766.3 ℃ after the compression.

So, actually this is not a heater this we can write as a cooler, because it has cooled, it has cooled the flow, it has reduced the temperature from 766.3 to 500 ℃ and everywhere it is in vapour phase, so vapour is 1, so for the time being let us make it off just to save the clutter and what is the next, so it is written a Chiller-flash combination are used at the downstream of the reactor.

So, we have done up to this point. So, from here to here we will have a Chiller and a flash. Let us use a Chiller over here and a flash. So, let us write C_2 and then flash 1 and attach these 2. Now press next, it is asking the heater inputs, now pressure we know that there is no pressure drop; until unless the reaction at the second reactor takes place. So, we just write 0 over here but we do not know the temperature.

So, for the time being, let us give a temperature, say 50 ℃, and press next and ask for the flash well it is said the flash tanks are operated at zero duty, so the pressure drop is 0 and duty of the flash that is also 0. Now it is ready to run. So, run is complete. Let us check the flash outlet, so go to f_1 and see the stream result. Before that, just give a name, let us name this one as C_2 out, let us name it f_1 wrap and this is f_1 liquid, it is said the Chillers are set.

So, the minimum amount of water in the first flash tank escapes through the vapour stream of the flash tank. So, we have to set a minimum amount of water through f_1 vap. Now let us check how much vapour has gone through f_1 wrap? For that go to the stream, so it is said that out of 115.679 kmol/hr only 0.82254 kmol/hr of water is going through f_1 vap.

But if you want it to reduce more, if you say that no, I want to send even less than that for that, you have to use a design spec. So, design spec is kept over here, so this is your design spec and you can write say WATFLOW, and this is a mole flow type in the stream f_1 vap of component water. So, you want to minimize WATFLOW and the identity of the word flow you have given it is mole flow of water in stream f_1 vap unit is kmol/hr.

Let us give a spec, so you can just write WATFLOW over here or in general there will be plenty of such variable you have defined then what you can do you can just right click and check the variable list, all those variables which you have defined they will be visible over here. You can just drag that variable over here and keep it. So, this is one way of putting the spec over there. If you remember the name, you can directly write w a t f l o w, but if you have a lot of defined variables you have to search, then you can use this way.

Now ideally, you never know what the value should be, but you say my target is 0, which means I do not want any water to flow. But you have to give some tolerance because ideal 0 will never be possible in any aspen plus calculation. So, you have to give some tolerance, say give a tolerance of 0.1, so any value below 0.1 will be acceptable to you. So, you define the spec.

Now you have to vary something by which you can attain the target and what you can vary? You have to vary this 50 °C because this temperature we never knew, the Chiller temperature we never knew. I have just given a value, but you want the simulation to vary this number until the target is achieved. So, it is a block variable which block C_2 block, the variable is temperature.

Now you give a lower limit of 0 and an upper limit of 100. You never know where it will reach. Just give a range; you hope that the value will be reached within this upper and lower limit. Now give a name to this block write as ds 1. So, design spec 1, ready to run, so just run it. So, it has run, check the result, it has come to 4.32721 centigrade. That means it started at 50 ℃ because that is the value that we have given.

And it has started doing the simulation and reached this point because here it has reached our target value, it has come below the tolerance limit of 0.1 at temperature 4.32. So, at that temperature, the water flow will be below 0.1. So, you can check the stream result once again, check the stream result, so earlier we had some 0.82 something, now it is 0.005. So, the almost entire amount of water has gone to the liquid line, only a small amount of water goes up.

So, you can just reduce the tolerance value, it might or it might not reach because it is some sort of optimization routine that will work in aspen plus domain, you can never expect that whatever the target you want to achieve the optimization routine will be able to meet the target. Still, you can give some reasonable value, and I believe you will reach the target. You can see the mole fraction of water in the vapour line, it is very, very small so you can argue that your f_1 vap is moisture-free which is a requirement for the second reactor.

So, now let us go to the second reactor condition. For that, let us go to f_1 vap will pass through a heater and then one reactor and then one heater and flash in between there will be a valve which will be depressurized from 55 atm to 10 bar. So, let us keep them so that we will place a heater first. So, place a heater then we will place a reactor, then there is a pressure changer, then there will be a another exchanger and finally there will be a flash tank.

So, let us write it as heater 2, so actually, there is no heater till now so we can write heater one no problem, and this is a misnomer it should be C_1 out and we can write it as CSTR2, this one is val 1, this one is Chiller. So, it should be Chiller 3 and this is flash 2. So, connect this with this one, material stream connection, this to this, this to this, this to this and finally this to this.

Now here also the idea will be somewhat similar. As you understand, the temperature of f_1 vap calculated by design spec is significantly, very less, it was 4 point something ℃, so it is very low. But the CSTR operates at 227 ℃. So, we have to increase the temperature with this heater. So, heater specs you can write as 227 ℃ and 0 bar no pressure drop.

So, this is H1 out, then CSTR it will be 0 bar, no pressure drop, temperature 227, valid phases vapour only and reactor volume 12000 liters or 12 m^3, the kinetics, the r_2 is waiting for you just use it and your CSTR2 is set. So, write here as r_2 out and here v_1 out and this one is c_3. Now again we do not know the temperature of the c_3 because we have to set this Chiller temperature to minimize the methanol loss with the second flash tank.

We have defined water-free or moisture-free movement of the f_1 vapour, similarly, we have to ensure methanol free movement of f_2 vapour. But for the time being, let us say that we do not know the temperature. Let us say our temperature is 50 we will do it later, and the zero pressure drops, so we have set it valve, valve we have to set outlet pressure as 10 bar. Because until this point until the output of CSTR2 there was no pressure drop, it started at 55 atm over here.

So, it began from 55 atm it was running at 55 atm all through. At this point it should have 10 bar pressure because without reducing it we cannot run the flash, there are certain process constraints. So, the valve is set at 10 bar and finally, the flash tank will have zero pressure drop and zero duty. So, both zero and zero. So, all set it is ready to run. So, please run and now check the stream result of we have not set the so we write f_2 vap over here and f_2 liq over here, and you write C_3 out over here.

Now just go to stream result, yes, so check the molar flow f_2 vap is having 1.27512 kilomoles per hour and we are not happy with this, so we want to reduce it. Now let us try to reduce and again the same strategy we will set another design spec over here, this block name is DS2 and you set it as define methanol loss in the line, which is again a molar flow type of stream f_2 vap of component methanol then spec.

So, check the variable list, we have methanol loss, target 0, and give a tolerance 0.1 what you need to vary? You have to vary the C_3 temperature. So, type block variable which blocks C_3, variable temperature lower limit set 0, an upper limit set 100. Let us check what happens. Run it, well so go to results of ds 2. So, it targets 6.60 ℃ where it is going below 0.1.

So, if you now go to the f_2, f_2 streams instead of 1.2, something that you have seen before, you can see almost the entire methanol is going to f_2 liquid, only 0.088 kmol/hr is going through this line. Mole fraction you can see the mole fraction of methanol is 0.002, which is very, very less. Now the time has come for us to check what the actual product of these reactions is?

So, you compare it with the original feed that we have sent. So, the entire line we have it began from feed one f_1 liquid is coming from here, this is the only feed in the system f_1 liq is coming through this, f_2 liq is coming through this and f_2 vap is coming out. So, we have 1 feed and 3 outputs. So, let us go to stream results over here and add 2 more lines, one is f_1 liq, no let us check it feed, and this one is f_1 liq.

Now please analyze. So, initially, we began with 500 kmol/hr of which 125 kmol/hr was carbon dioxide and 375 kmol/hr of hydrogen. In the first reactor, we had to throw 115.625 kilomole per water that we had to throw, and we are not unhappy with this because it is just water it is not our product. But we lost 0.321742 kmol/hr of hydrogen and around 2.69 and 2.93 kmol/hr of carbon monoxide and carbon dioxide, respectively.

Now, this we could not help because 115 kmol/hr of water will have some solubility, and carbon monoxide, carbon dioxide, and hydrogen will be soluble, which is why it is going. So, we really cannot help. Anyway, that is the part of the process we cannot help much. What about f_2 liquid? F_2 liquid will have 39.3497 dimethyl ether which is our product. So, this we have to keep. So, actually f_2 liquid is our product line.

But here we have water and methanol 2 and fortunately, we do not have much of carbon monoxide and hydrogen in this line, carbon dioxide is there, it will probably be dissolved into water. But obviously, we have methanol which is a product that is of use. So, we have to have some means to separate water and methanol and make use of methanol that we will learn later. For the time being, let us check this f_2 vap line.

And here, we have 33 kmol/hr of hydrogen, which we cannot throw .We also have some carbon dioxide and very little carbon monoxide, but hydrogen is 33 kmol/hr, which is a big amount we really cannot throw. So, we want to recycle this stream. So, at this moment our goal is to recycle f_2 vap. For that, let us again go back to our system.

Now let us check what the temperature and pressure is over here? So, the temperature is 6.6 °C, and the pressure is 10 bar. We definitely do not want to recycle everything over here, we will rather split at this point into 2 streams say 10% of the stream will be purged, and the rest of the 90% will be sent to the CSTR. Now the question is where exactly will throw it? Whether we will throw it at CSTR at this line, this point or this point or this point where exactly we will add?

Now, remember the pressure is 10 bar, and here, from this point to this point entire line we have 55.7 bar. So, if we just add it the flow will be in this side, we will not be able to put it over here. So, either we have to use a compressor at this point, pressurize it to 55.7 bar and feed into the line, or we can put a valve over here and release the pressure to 1 atm. So, from 10 atm to 1 atm and this line add to the feed line.

Because the feed line is coming at 1 atm, this line will also come and this flow will also come at 1 atm and here we can use a mixer and then the entire thing can be compressed through this compressor. If you do this way, the capital cost will increase because you have to use an extra compressor over here. But if you go this way, you have to depressurize to 1 atm and then again compress it will have a recurring cost.

So, you have to decide whether you will go by depressurizing and using a mixer or pressurizing from 10 atm to 55 atm and then attach with this line that decision as a process engineer you have to check by analyzing the cost, etcetera. For the time being, let us take this path that we first depressurize and then attach it to the feed line. So, we shall use a splitter over here. So, just put it over here and let us use a mixer over here.

So, rename them splitter and mixer. And also, we will have a pressure changer that is a valve. So, here we will say valve 2, and this one, we will rotate the icon from this side to this side. Otherwise, it will look in this manner. So, we want from this side to this side or else what we can do; we can flip this way and this way. Now attach it to this side, take it here and material out this to this, this to this.

And there will be another connection, so this one we will send it this, so this is purge, this is splitter out and this is v_2 out and this one we have to reconnect destination to this point. So, basically, we will have and will attach them m out. So, now it is set, so first splitter will split purge to 10%. So, it is written in the problem statement that 10% of the vapour outlet of the second flash is purged while the remaining portion is depressurized to atmospheric condition.

So, 10% purged 90% will go over here and it will be depressurized to 1 atm and it is done. Now it is ready to run, so run it, so thankfully it has converged, so sometimes recycle does not converge in that case we have to be a bit careful but here the ds 2 fails. What is ds 2? Ds 2 is the design spec 2 where we wanted to reduce this line f_2 below a certain limit. So, here it is not able to bring it below 0.1.

So, it is going up to 0.23, so what exactly did we do with ds 2? With DS2 we wanted to minimize methanol loss through this line by tuning the temperature of $C_{3,}$ and we got a good result because it went down to 0.1. But after we added the recycle stream, the amount of input has increased, so the ds 2 is not able to converge below 0.1. But do we really think that the methanol is being lost over here?

Methanol is lost in this line not in this line because methanol is coming back to the system. So, we have to change the DS2 and tell them that I do not mind if f_2 has more than 0.1 but purge line should have below 0.1. So, that is my goal. So, change DS2 accordingly instead of f_2 vap we set purge. So, in the purge line the methanol loss should be less than 0.1. So, reset to the original and then run it once again and check whether DS2 is satisfied.

Yes now DS2 does not fail. So, what is the condition at purge? We find over here the purge line the methanol loss is below 0.1, only 0.07 kilomoles per hour. So, below 0.1, and we are happy with this. So, with design specs, we know how to do it. So, we have learned all the blocks and all these lines, their stream lines they are all done. Now our job is not over because this f_2 liq lets us remember f_2 liq contains, as we discussed before, f_2 liq contains so much water-methanol in DME.

So, we have to do something with this. Now let us see with added recycle stream what changes it has made to f_2 liq. So, go to mole flow, and we find 26.2378 kmol/hr of DME, water is almost twice the methanol, and thankfully there is almost no CO and minimal amount of CO 2 and hydrogen is also very small. So, let us use a separator over here to separate three streams.

So, we will have a separator, and this separator will have one input and there will be three outputs. So, let us be a membrane separator, and this membrane separator separates all the gases DME and other liquids. Liquids means the methanol and water solution. So, we define membrane separators as gases that will have CO, CO_2, and hydrogen. And then DME line will have full DME all other 0.

Gases will also have all other line 0. So, it is completely defined because we do not have to say anything about liquid because liquid line automatically will have water and methanol. So, this membrane separator if we run and check the line streams of membrane separations and you will find, DME will have only 26.2378 DME, the liquid line will have water and methanol, and gases will have CO, CO_2 and hydrogen.

Now we have to work with this liquid line, because it has water and methanol. Now the best way of separating water and methanol is by distillation only. So, is it a very good condition for distillation, it is having 10 bar pressure and 17 °C temperature, first release the pressure and see what temperature it goes to, so this is valve 3, and this is v_3 out and valve output let us say 1 atm.

It is always better to distillate 1 atm pressure or say 1.1 atm and run it. So, we have got 17 °C only, so the temperature has not changed. **(Video Ends: 1:09:42)** So, what we can do is we can attach a distillation column over here. Now you already know what the procedure is. I do not want to do it I want to keep it for you to practice from this point onwards how to separate methanol and water. Just to recapitulate what you can do.

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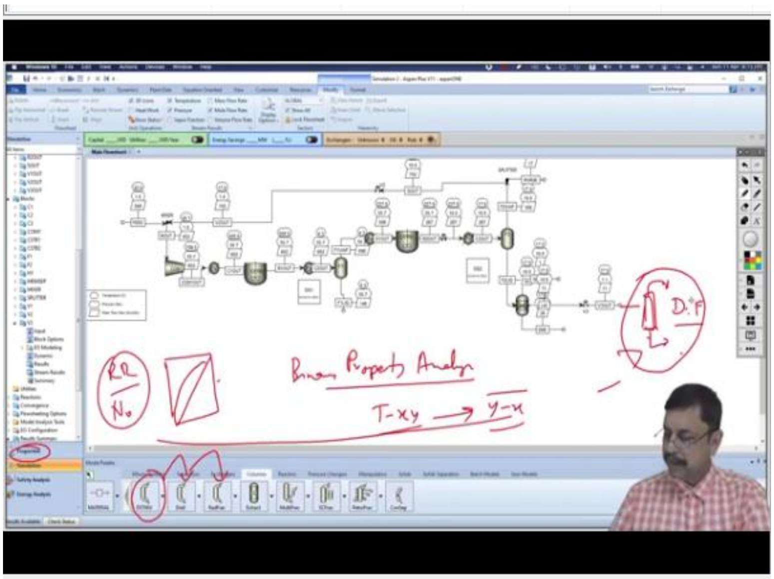

So, basically, you have to begin from here, so your distillation column will be somewhere here like this. Now the best way of doing is to begin from DSTW, so first you use DSTW over here, this is the shortcut distillation method and even before using DSTW you have to go to the property analysis and there you have to use the binary analysis tool, there you have to use T-xy diagram.

From there you will get y-x diagram and y-x diagram will give you the idea about what could be the minimum reflux ratio, from there you can have a minimum number of stages. So, in shortcut distillation method, either you have to provide reflux ratio or number of stages both this information you can have from this y-x diagram, rough idea that you will have and if you give this information over here DSTW it will give you the display to feed ratio and then minimum number of stages, minimum reflex ratio DSTW will calculate all those information.

And then you can replace it by distl and finally you can use RADFRAC. So, I am not doing it here. I leave it to you for practice and I believe you can take it from this point onwards because this has been discussed many times in the previous case studies. With that we come to the end of this lecture; we shall take up a new case study in the next lecture; till then goodbye.