

Aspen Plus Simulation Software – A Basic Course for Beginners
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Lecture-24
Synthesis of Methanol from Syngas

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(Refer Slide Time: 00:35)

Case Study – Synthesis of methanol from syngas

Methanol needs to be synthesized from 1000 kmol/h syngas, consisting of 6% CO, 27% CO₂, and 67% H₂, at 60 °C and 1 atm pressure. An isothermal equilibrium based CSTR of size (4.5 m³) will be used which will operate at 45 bar and 280 °C. The reactor will be governed by the following equilibrium reaction kinetics:

$$\text{CO} + 2\text{H}_2 \rightleftharpoons \text{CH}_3\text{OH} \quad (1)$$

$$\text{CO}_2 + 3\text{H}_2 \rightleftharpoons \text{CH}_3\text{OH} + \text{H}_2\text{O} \quad (2)$$

and supported by water-gas shift reaction:

$$\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2 \quad (3)$$

The equilibrium constants of the above reactions are given by the following:

$$\left. \begin{aligned} \ln k_{1,eq} &= -29.03 + \frac{11820}{T} \\ \ln k_{2,eq} &= -24.36 + \frac{7052}{T} \\ \ln k_{3,eq} &= -4.67 + \frac{477}{T} \end{aligned} \right\}$$

Handwritten notes on the slide include:

- ①
- ②
- $A = \ln(k)$
- $B = -\frac{E}{R}$
- $\ln k_{eq} = A + \frac{B}{T} + C \ln(T) + DT$
- $k_{eq} = K \frac{E}{RT}$

In today's lecture we shall perform a case study on synthesis of methanol from syngas that means synthetic gas. Now the problem statement is something like this, the methanol needs to be synthesized from a 1000 kmol/hr syngas consisting of 6 mole percent CO, 27 mole percent CO₂ and 67 mole percent of H₂. And the syngas, the mixture is at 60 °C and 1 atmosphere pressure. Now the reaction will take place in an isothermal equilibrium based CSTR of size 4.5 metre cube that means 4500 liters.

It will be used and it will operate at 45 bar pressure and 280 °C. Now this reactor will be governed by the following equilibrium reaction kinetics. Here both CO and CO₂, they will react with H₂ to form methanol and water. So, these are the parallel reactions that will happen for production of methanol. And these 2 reactions will be supported by water gas shift reaction where CO reacts with water at certain temperature and pressure to form CO₂ and H₂.

And this H₂ will aid to methanol production. The equilibrium constants of above reactions are given by the following. Actually, the equilibrium constant is given by this equation, but in Aspen we do not have the

opportunity to give the reaction constant in this form rather it takes the form of logarithmic of k equivalent = $A + B \ln T + C/T + D$.

$$k_{eq} = ke^{-E/RT}, \ln k_{eq} = A + \frac{B}{T} + C \ln(T) + DT$$

$A = \ln k$, $B = E$ (Activation energy), $C = R$ (Universal gas constant)

So, that is the equation with A, B, C, D this constants Aspen plus desires to have to run the simulation.

So, we have to give A, B, C and D, this particular equation can be formed into this format, it is simple, just take a logarithmic of both sides, you will get these values. Where obviously you know the A will be ln of k and B will be the activation energy and the universal gas constant, they will be given. Now these are the parameters that one can find from experimental studies but we will perform this simulation in 2 ways. In the first case we will not use them, we shall let Aspen do the calculation based on the idea of minimization of Gibbs free energy of formation.

Because we know for any spontaneous reaction the Gibbs free energy of formation will be minimized. So, we will ask Aspen to do it, that way, so Aspen will calculate and try to find out the minimum Gibbs free energy. And the second case we shall use all of them because we do have the experimental results for that which are given in these 3 equations.

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Case Study - Synthesis of methanol from syngas

Methanol needs to be synthesized from 1000 kmol/h syngas, consisting of 6% CO, 27% CO₂, and 67% H₂, at 60 °C and 1 atm pressure. An isothermal equilibrium based CSTR of size 4.5 m³ will be used which will operate at 45 bar and 280 °C. The reactor will be governed by the following equilibrium reaction kinetics:

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$$\ln k_{3,eq} = -4.67 + \frac{477}{T}$$

Handwritten red annotations: 'A, B' next to the first two equations, and 'C, D, X' next to the third equation.

So, the values of A and B, they are given over here for all 3 reactions, this is for this reaction, this is for this reaction and the third one is for water gas shift reaction, for all of them C and D are 0. So, we shall use this but as a second case.

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A membrane separator, operating at 60°C and 12 bar pressure, will be employed to separate the liquid and vapour. The liquid will be distilled at 1.6 reflux ratio and 1.6 bar inlet pressure to recover methanol, while the vapour will be passed through another membrane separator, operating at 280°C and 45 bar pressure, to separate H_2 and recycle it back to the reactor. A simple mixer unit will be used for recycling purpose.

For distillation of methanol, a DSTWU unit will be used for shortcut calculation followed by "RADFRAC" column for more rigorous calculation.

We possess one isentropic compressor with 90% isentropic and 80% mechanical efficiencies at our disposal. We also have a second isentropic compressor (using ASME method) with 70% isentropic and 80% mechanical efficiencies that can be used for our work.

We have two valves which work as "adiabatic flash for specified outlet pressure". We also have three simple exchangers which can be used as a heater or cooler, as and when the need arises.

Handwritten notes on the slide: CO , CO_2 , H_2 (left); Methanol, W.L. (right).

Then after the reaction there will be a membrane separator which will operate at 60°C and 12 work pressure and it will be employed to separate the liquid and vapour. The liquid will be distilled at 1.6 reflex ratio and 1.6 bar inlet pressure to recover methanol. Because the liquid will be a mixture of methanol and water, while the vapour which actually will be a mixture of unreacted CO , CO_2 and H_2 . They will be pass through another membrane separator operating at 280°C and 45 bar pressures to separate H_2 and recycle it back to the reactor.

H_2 is a valuable component, so we should not lose it, so we will recycle it back to the reactor. And a simple mixture unit will be used for recycling purpose. Now as you may understand that we have several temperature and pressure figures over here, different units they operate at different pressure and temperature. So, we shall use other unit operations like heater, cooler or pressure changers as per the requirement in order to get those required pressure and temperature for those units.

Now for distillation of methanol, first we will use a DSTWU unit which will be used for shortcut calculation. In the last lecture we have seen how DSTWU and distill unit has been used for BTX column. Now the same thing will be used over here, we will not use distill unit but we will use DSTWU for shortcut calculation. And then by taking the result we will continue our calculation with Radfrac column for more rigorous calculation and more accurate calculation of the methanol recovery.

Now as I said that we will need the pressure changers and other unit operations, so we possess 1 isentropic compressor with 90% isentropic and 80 mechanical efficiencies. And we also have a second isentropic compressor which will be used using ASME method and it has different efficiencies for isentropic and mechanical operations and they can be used for our work. And we also have 2 valves which work as adiabatic flash for specified outlet pressure.

And we also have 3 simple exchangers which can be used as heater or cooler and we can use them as the need arises. So, we shall be using all of them let us see how.

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So, in order to do the simulation, let us go to the Aspen simulation window. So, first we have to insert the component ID's, so first it will be CO, CO₂, H₂, methanol and water. So, these are common chemicals and if you just write the chemical formula of those components, it will be identified by Aspen very easily. Now we shall use PSRK method for this predictive Redlich Kwong Soave equation of state for this kind of system.

Now press next, it is yet to calculate the binary interaction, run it again, yes, the operation is done, now go to the simulation window. Now we have a feed line and the specification of this feed line is, we can refer to the problem statement it is at 60 °C and 1 atmosphere pressure. So, 60 °C and 1 atmosphere pressure and total is 1000 kmol/hr syngas of which 6% is CO, 27% CO₂ and 67% H₂. So, out of 1000 kilomole, we have 60 kilomole of CO, 270 of CO₂ and 670 kilomole for H₂, so just directly we can write those numbers.

So, we write here 60, here we write 270 and here we write 670, total we have 1000 kmol/hr. So, we have this feed line, which is at 60 °C and 1 atmosphere pressure. But at the same time, we know that the equilibrium based CSTR operates at 45 bar pressure and 280 °C. So, we have to pressurize the feed before we feed into the reactor and this is vapour phase because all of them are CO, CO₂ and H₂ at this temperature and pressure it will be gaseous form. So, we have to use a compressor.

And as we know that we have 1 isentropic compressor with 90% isentropic and 80 mechanical efficiencies at our disposal, let us use it. So, for that we bring in a compressor write COM1 OUT. So, compressor 1 output and run the simulation before that we have to say what type of compressor it is? It is an isentropic compressor with 90% isentropic efficiency and 80% mechanical efficiency that is stated in the problem statement.

So, once we give this value, we have to specify the discharge pressure. Now we need 45 bar because our problem statement says that CSTR operates at 45 bar, so we have to write 45 bar is the discharge pressure. Now run it, yes, now you can see the result, stream result, so what is the temperature of COM1 OUT? So, because we have pressurized the temperature will also increase as the pressure increases the temperature will also increase. And the temperature is now 629 °C but our reactor operates at 280 °C, so we have to cool down.

We have to cool down without compromising with the pressure. So, for that we shall use a simple heater or we have to set it as a cooler because for heater and cooler we have the same model in Aspen plus. Now let us give a name, so it is renamed as COM1 and let us rename it as heat 1 or write as H1, we have 3 heaters like that

attach with this and attach like that and let us write H1 OUT. Press next, so temperature of the heater will be 280 °C because that is the temperature is required for the isothermal reactor.

And the pressure we do not compromise we just write 45 bar pressure. So, once we run then our outlet temperature and pressure of heater is suitable for operation in the reactor. So, we are ready to use the reactor for our need. So, we simply attach a reactor, we need a CSTR, so place a CSTR over here, connect it out, rename them as reactor this you can write as R OUT, press next. So, we have to give lot of information from the reactor obviously we know them. First of all, we have to set the pressure of the reactor 45 bar, temperature of the reactor 280 °C and the valid phases will be vapour only.

Because if you see the vapour fraction it is 1 over here, vapour fraction is 1, that means the entire input that is going in it will be in a vapour phase. So, the reaction will occur in vapour phase only, so it will be vapour only not liquid. And the reactor volume, it is 4.5 metre cube, so it is 4.5 cubic metre and then we have to go to kinetics, we have not yet defined any kinetics till now. So, we have to press new and this reaction set R1 which is obviously general type, press ok and R1 is selected.

Now we have to set R1 right, so go to R1, create new, it is an isothermal equilibrium reactor, so the reaction will be of equilibrium type. So, we have to give all 3 reactions, so reaction 1, reaction 2, reaction 3, so all 3 reactions we have to give. So,

first reaction is $\text{CO} + 2 \text{H}_2 \rightarrow \text{CH}_3\text{OH}$,

so, write reaction 1, it is name, the components are so, this is 1 mole of CO reacts with 2 moles of H 2 to form 1 mole of CH₃OH, so the first reaction is done.

Similarly, we have to write the second reaction, again it will be equilibrium reaction, write reaction 2 which will be CO₂ just refer it once again $\text{CO}_2 + 3\text{H}_2 \rightarrow \text{methanol} + \text{water}$. So, CO₂ 1, H₂ 3 to form CH₃OH 1 and water 1, so the second reaction is done and finally the third reaction also we have to do in the similar manner and this is the water gas shift reaction, please refer again

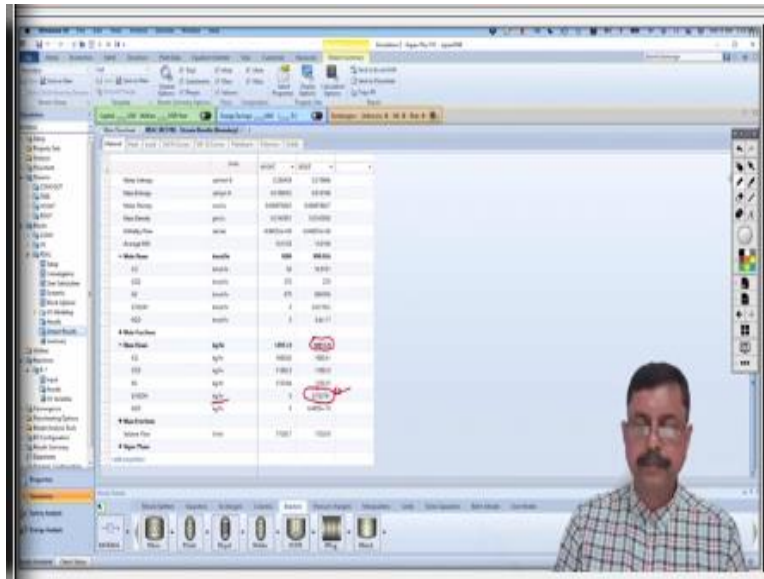
$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$

so, all of them are 1, so all the reactions are given.

Now as I said that we shall do it in 2 ways. In the first case we will ask Aspen plus to compute k equilibrium from Gibb's energy. That means the Aspen will try to minimize the Gibbs energy of formation, it will minimize and then it will give us the result, so let the calculation be done by Aspen plus. So, we leave it over here, we will just change the liquid to vapour because the reaction is not happening in liquid phase, reaction is happening only in vapour phase. So, we have to write vapour and temperature approach to equilibrium, I believe it will

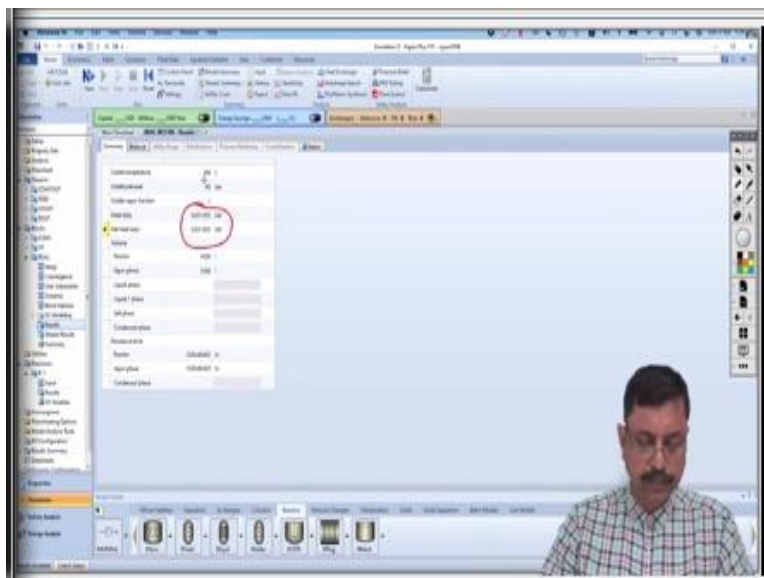
be taking place at 280 °C because we have been asked to operate the reactor at 280 °C. So, now it is ready to run, so press run and it has run very quickly, just go and see the results of reactor output.

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The amount of methanol produced is only 0.702781 kg/hr out of the total mass flow of 14 or 15000 kg/hr the amount of methanol is this much and we are not at all happy with this kind of result. So, let us now dig out why we are not getting this result? For that first let us go and check the other results.

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Now we can see the heat duty is very small, we know it is an exothermic reaction, so the value of heat duty will definitely be negative but we do not expect the value to be so small. I strongly believe that Aspen's calculation on the basis of Gibbs free energy minimization is erroneous. So, we do not leave this calculation on Aspen rather we shall input the experimentally found parameters of A and B in the k equilibrium equation

as shown before and redo the computation of reactor performance. For that we shall go back to the reaction input and edit it and go to equilibrium instead of compute k equation from Gibbs free energy we will say compute k equilibrium from built in expression. And here you can see the built-in expression, it is log of k equilibrium = A + B by T + C ln T + DT where T is in Kelvin.

$$\ln k_{eq} = A + \frac{B}{T} + C \ln(T) + DT, \text{ where } T \text{ is in Kelvin}$$

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So, we have to give the values of A, B, C and D and we already have the information in our problem statement, so we can use it. But what is this key basis? Now for that let us see the options, we have so many key basis, mole gamma, molal gamma, mole fraction, mass fraction etcetera, we shall use fugacity. Because here equilibrium constant is product fugacity to the power stoichiometric coefficient and entire reaction is happening in gas phase, so it is better to use fugacity.

Now we shall again refer to the equilibrium constants for above reactions and we find the following. So, the first reaction A = -29.03 and the value of B = 11820, so it is -29.03 and B is 11820. So, this is for the first reaction CO and H₂ produces CH₃OH. Let us go to the second reaction, here also we have to change it to vapor and 280 °C, compute k equilibrium from built in expression, key basis which is fugacity, the value of A in this case -24.36 and B will be 7052.

And third reaction again it will be vapor phase 280 °C fugacity and the key basis -4.67 and B = 477, so we are done with the option for computing k equilibrium from built in expression. So, this k equilibrium will be used for all the reactions from now onwards. So, run, so the results are now available; now let us go to check the

stream results. And here you can find the molar flow rate, you have 143.863 kmol/hr. Now compare to the case when you asked Aspen to calculate the K equivalent based on the Gibbs free energy minimization.

At that time, we did not have almost no production of methanol but with correct information given to Aspen we have achieved a better performance from Aspen. So, this gives an idea that you have to insert as much information as possible from your side based on your experimental data or from literature or whatever. As much realistic information you give to Aspen, it will be better for it, because if you leave everything to Aspen to do then it will probably not be able to perform at the expected level.

So, we have got the reactor output, now it is again the vapour fraction is 1, I think the entire system is working in the vapour mode, we just switch up the vapour fraction information, it will just create a clutter, we will bring it back whenever necessary. So, we have a reactor output at 280 °C and 45 bar pressure. Now let us check what else is said? A membrane separator operating at 60 °C and 12 bar pressure will be employed to separate the liquid and vapour.

So, the membrane separator will work at 60 °C and 12 bar pressures, whereas we have the reactor outlet at 280 and 45 bar pressure. So, definitely we need to depressurize, now for depressurizing we do have to use a valve. So, let us use a valve over here, so we connect this valve and there is a valve outlet, so rename the valve as say V1 and this is V1 OUT and press next. Here the outlet pressure of the valve obviously 12 bar because that is expected.

And as we have seen in the problem statement, we have 2 valves which work as adiabatic flash or specified outlet pressure, so that is the one which we are using, adiabatic flash for specified outlet pressure. So, just run it and you can see the stream results, this is V1 out. And the V1 OUT, pressure is 12 bar but the temperature is 262 °C, from 280 to 262 but the membrane separator operates at 60 °C. So, we have to use another cooler over here, so just take the cooler, so attach a cooler.

So, rename it as H₂ although it is a cooler but we can simply name it as we wish and then outlet of this cooler will be H₂ OUT. Now let us check, so the information about H₂, we need a temperature of 60 °C. So, write 60 and pressure remains 12 bar or here we can say pressure is 0, that means there is no pressure drop, 0 bar means it is not vacuum the heater will not work at vacuum. As we said any value 0 or less it indicates pressure drop not the absolute pressure.

We have reduced the temperature to 60 degree, from 261 or something we are reducing to 60 °C. So, run it and check the value here, it is 60 °C and 12 bar. Now if you want to show the heater work, you can see how much of heat we need to throw out? It is 1398614, so for the time being let us use SI unit to check, it is so many

watts, so 1, 2, 3, 4, 5, 6, 5.8 megawatt of heat we have to check out in order to decrease it from 535 Kelvin(K) to 333 Kelvin(K).

Here also we have to take out 3.4 megawatt of energy in order to cool down from 902 Kelvin(K) to 553 Kelvin(K). Anyway, let us go back to our original unit set. Now this is ready for separation, so again it is a membrane separator, you remember in the past we have used another case study where you have used membrane separator probably for gas separation. So, we take a membrane separator, use the SEP model, it is again a black box kind of model, so attach this, then here 1 line and there will be another line like this.

So, if you check the vapour fraction then you will see here you will have a vapour fraction of 0.45, that means 45% of the material that is coming out of this H₂ and entering separator that will be vapour and 55% will be liquid. And we know the liquid will be mostly methanol and water because at 60 °C and 12 bar pressures only methanol and water will be in liquid form CO, CO₂ and H₂ they will not be in liquid form. So, we can write here as liquid and we can name them as vapour, now press next.

So, B3 separator let us rename them, do not keep it as B3 write SEP 1, so it is SEP 1, yes, so press next. So, it is asking from SEP 1 liquid stream. So, it is asking what do you want in the liquid stream. Obviously, I will want only methanol and water in the liquid stream, all other I want to throw it in the vapour stream, so CO, CO₂ and H₂O will go to vapour. So, we write 0, 0 and 0 over here, so there is no methanol and water that will go in the vapour phase, all of them will go to the liquid phase, so press next, yeah, so it is done.

Now you check this is liquid phase, so the vapour fraction is 0 over here, all is liquid because entire methanol and water we have thrown over here and here we will put a distillation column, but that will be later. And here entire vapour fraction, so it is 1.00, so this is the completely vapour. Now this vapour has to be separated because it contains if you see the output of separator 1 you can see in the vapour line it will contain only CO, CO₂ and H₂, so H₂ has to be separated.

And for that we have a second membrane separator and that separator will work at 280 °C and 45 bar pressure to separate H₂. Now why it is operating at 280 °C and 45 bar pressure? Because the outlet of this separator will go to the mixer and it will be recycled back. So, as the reactor pressure is 280 °C and 45 bar pressure, you can check it is 280 °C and 45 bar pressure, so the membrane separator over here which will throw out the unreacted H₂ that will also operate at 280 degrees C 45 bar pressure.

But we have 60 degrees C and 12 bar pressure over here. So, we have to first pressurize from 12 bar pressure to 45 bar pressure. Then again, we have to use the second compressor that was with us for our disposal. We have our second compressor; we have also a second isentropic compressor using ASME method with 70%

isentropic and 80 mechanical efficiencies, so we will use this one over here. So, first let us flip it, so that we can connect it in this manner and the outlet of this we can throw it this side.

Now again we have to rename this, so rename it as COM2 compressor 2 and this will be COM2 OUT, press next, so the compressor you have to press the type isentropic using ASME method using 70% isentropic efficiency and 80% mechanical efficiency as stated in the problem. And we can use any one of them, discharge pressure, pressure increase, pressure ratio, power required, so we have used discharge pressure before. At this moment let us use something else, now here it is 12 bar pressure, we have to bring it to 45 bars.

So, it is slightly less than the 4 times, so what we will do? We will use pressure ratio and we use 4 here. So, that whatever the pressure it is coming in it will multiply with 4 and that will be the outlet pressure of the compressor. So, let us run and check. So, you can see the outlet pressure is 48 bar, so from 12 bar to 48 bar because we have used pressure ratio of 4, so this much of work has been done. Now for the timing let us put it off and vapour fraction also we will put it off because we know where the vapour is going and where the liquid is going, the entire portion is vapour only this part is liquid.

So, we are at 48 bar pressure and 287 °C but we have to reduce it down to 280 °C, it is 287 °C. So, we have to use the 3rd heater that is with us, now let us flip it and then connect it and again throw it out, yeah. Now rename them, it is our heater 3 and then this will be H3 OUT and this one, press next. So, again the heater temperature should be 280 and pressure will be 45 bar, run, yes, so the outlet pressure is 45 bar and temperature is 280 °C.

Now for that how much work it has to do, just go and check it is 4413 cal/sec work has to be done. Now this is ready to separate, now we have to bring in the second membrane separator that we have. And the second membrane separator, it will separate H₂ and CO, CO₂. So, we bring in the second separator, let us use this one and again we have to flip them, enter, exit and there will be a second exit. So, you have to rename, rename it as SEP2, keep it here.

This one let us write CO and CO₂ because we know this stream will take CO and CO₂ out, whereas this stream will be purely H₂. So, H₂ name already exist for this block, so this name is not taking this name, we write so H₂ is taken. So, press next, outlet stream H₂ will give 1, that means the entire H₂ has to be separated all other will be 0, CH₃OH and water anywhere they are not here but other 2 were there that we have knocked off.

So, now it is ready to run, so run it and check the stream result of separator 2 and you will find in the H₂ line, it will be only H₂ and CO, CO₂ line will be like this. Now this particular H₂ has to be recycled back over here. Now here you have to insert one mixer because in the mixture they will be H1 out and they will be Hight both will be mixed. So, for that what you need to do is you have to select this line and then you have to press insert.

Reconcile stream H1 OUT before inserting the block you have to say yes. And then copy results from input specification and enter the name of block ID, so write mix, it is a common type, so say mixer and press ok. So, it is asking for the temperature estimate and all, you do not have to give anything just go by default. So, nicely it has brought in a mixture just check, it has nicely put in 1 mixer. So, you can just select them and bring it over here, so that you can have some more room.

This one you can change the icon, yeah, I like this icon. So, we rename it as R IN reactor in and this one we rename it as H1 OUT that will be more logical. Now we have to add this one over here, so you have a mixer which mixes H₂ and the outlet of heater 1 both are mixed and that becomes the reactor input. And this is at 280 °C 45 bar pressure; this is also at 20 °C 45 bar pressure, so there is no problem over here, just run once again.

Now before running let us check what is the amount of liquid over here. So, go to the stream leak and see the results, you have 143 kilomole of methanol and 264 kilomole water. So, just run and check whether it changes. So, now you have submitted the recycle and see how the value changes from 143 it jumped to 201, why? Because you have given the extra feed of H₂, so H₂ after recycling it has increased the methanol production, so that is the importance of recycling unused reactant or unused components.

So, we have got more amount of methanol over here, so we are happy. So, this part all the vapour phase part it worked fine for us. Now our job is not over, we have to separate methanol and water at this end because this is the liquid end. So, for that we have to use a column, so what is the strategy? Strategy says for distillation of methanol a DSTWU unit will be used for shortcut calculation followed by RADFRAC column for more rigorous calculation.

But we have to begin the way we have done in the previous case. Only thing is that this time in the property analysis we have to use binary analysis not pure component analysis. For binary analysis we shall use component 1 to be methanol, component 2 will be water the mole fraction 0 to 1 and pressure it will be 1.6 bar inlet pressure. So, we will use 1.6 bar over here and run the analysis, so in the T-xy diagram we do not find any azeotrope to be formed between methanol and water, so it is a straightforward case for distillation.

So, let us go back to the simulation and first we shall use a DSTWU because it is shortcut distillation, connect it and the material stream, this is liquid and vapour, rename it column vapour which will mainly contain the methanol part. And column liquid it will have mostly water and rename B 1 as column, now press next, the number of stages we do not know but the reflux ratio it is set. It is 1.6 reflux ratio; the liquid will be distilled at 1.6 reflux ratio and 1.6 bar inlet pressure.

So, reflux ratio is 1.6 and the pressure is also 1.6 the inlet condition, so the condenser will be slightly less said 1.5 and reboiler will be slightly more say 1.7. So, that will ensure that in our inlet if we give 1.6 bar inlet pressure DSTWU can handle that. So, what is the light key? Obviously, methanol recovery, well it is said that liquid will be distilled to recover methanol but it has not given any figure, that I have to recover 95% or 96% or 99.

So, let us be a little bit conservative, we will use 95% recovery at the very first instant, let us go for 95 recovery. So, write 0.95 and let us give water at say 0.05 water or we can write 196 also, not a problem and here we can give 4%. Let us see what happens? If required we can change it later, so run, yeah so results are available go and check the results, the stream results. So, C vap. the mole fraction it is 947.624, so it is not even 95%, so perhaps the reflux ratio is not enough.

So, let us change the reflux ratio say 3 and let us change the recovery to 98%, let it be like this or let it change it to much less say 01, run. Now see, mole fraction, yeah now we have got 98.6%, so we are happy that we are getting more than 96%. So, at this moment we need these results, so minimum reflux ratio and actual reflux ratio is 3, minimum number of stages, actual number of stages 9 will take, feed stage will be 7, number of actual stages above 6 and the heat duty in kilowatt or in say megawatt it will be 8.46 megawatt in reboiler and 8.08 in condenser.

The displayed feed fraction ratio is 4.42. Now we need this information for that let us snip it, so keep it for our later use, say done. Now go to this column, now this is DSTWU we do not need it, our shortcut calculation is over. So, we just delete this column and instead we bring radfrac because this is the one which we will use. In the last example we have used DISTL for BTX column example, today we will use radfrac, it is more rigorous.

So, we will connect it like this, this one will connect as a total condenser and this one will connect over here. ok Now it is hiding over here the name let us rename it as call again now one thing that you may notice that in both the cases it is written 2. But we have specified the condenser pressure is 1.5 and reboiler pressure as 1.7 but then why it is showing 2? Answer lies over here, you just press stream result, this icon you will see temperature and pressure there is 0 number of digits after the decimal point.

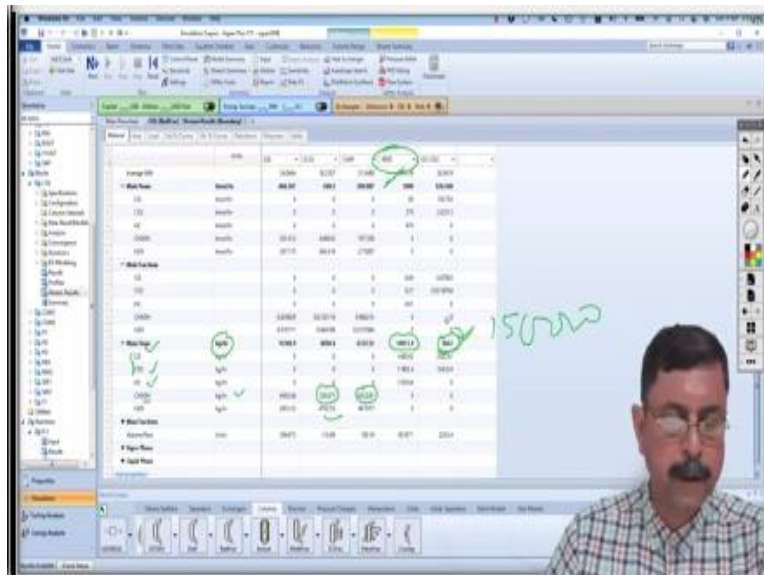
So, it is assuming a whole number, so instead if you write say 1 digit after decimal point for pressure. And if you say ok, then you see you will have 1.7 and 1.5 over here. So, without that it was approximating as a whole number, right now all these things are having one digit after the decimal point. So, sometimes it will be useful sometimes not, anyway so we have to complete the task, press next, obviously it is a calculation is equilibrium time number of stages.

So, so number of actual stages is 8.94, so let us take 9, total condenser type, vapor liquid, we do not know distillate rate but we know distillate to feed ratio which is 0.4269. So, let us write 0.427, so 0.427 and the reflux ratio is 3. Then go to streams, so the feed stream is above stage number, so number of actual stages above feed is 6, so it will be 9 - 6, so above 3. And then pressure, you write the condenser pressure 1.5, now others are optional, you may provide this optional information of stage 2 pressure, stage pressure drops, column pressure drops etcetera but there lies an issue.

Aspen will calculate the stage wise and column wise pressure drop based on the given information and while doing so it will try to match the feed stage pressure too. In case there is any problem in matching the feed stage pressure then Aspen will show some error message. Hence it is not advisable to provide pressure drop information unless the user is very much sure about that. Just directly run, yes, it ran successfully; now let us check the stream results in the column, yes.

So, C vap the mole fraction is, now it has reduced to 92%, now here from 98 to 92, so we are not happy. Let us increase the number of stages to 15 and feed stage somewhere around 6, let us try, just wild guess, so check the stream results. Here it has come to 0.986206, so ultimately what we get we get 197.328 kmol/hr of methanol that we can recover from this whole plant. So, in terms of kg/hr the mass flow.

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So, now we can see the feed line we have 14913.9 so nearly 15000 kg/hr of CO, CO₂ and H₂ we were feeding in the system, out of which we are recovering 6323 kg/hr methanol as our product. And 130.871 kg/hr of methanol is being wasted in the liquid line and 3647 kg/hr of CO and CO₂, they are becoming useless and they are being thrown out of the system. So, this is a huge number we can try to utilize it as a second recycle stream

and overall, this is our system. So, here we end our case study on methanol synthesis from syngas, so we end our lecture over here, thank you. (**Video Ends: 1:07:32**)