Aspen Plus Simulation Software – A Basic Course For Beginners

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

Lecture-22

Introduction to the Course and Basic principles of Image Formation

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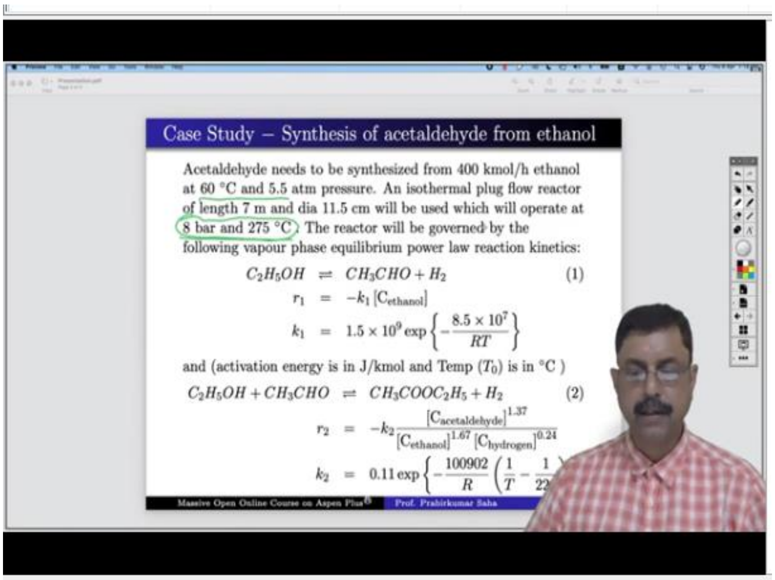

Case Study – Synthesis of acetaldehyde from ethanol

Acetaldehyde needs to be synthesized from 400 kmol/h ethanol at 60 °C and 5.5 atm pressure. An isothermal plug flow reactor of length 7 m and dia 11.5 cm will be used which will operate at 8 bar and 275 °C. The reactor will be governed by the following vapour phase equilibrium power law reaction kinetics:

$$C_2H_5OH \rightleftharpoons CH_3CHO + H_2 \qquad (1)$$

$$r_1 = -k_1\,[\mathrm{C_{ethanol}}]$$

$$k_1 = 1.5 \times 10^9 \exp\left\{-\frac{8.5 \times 10^7}{RT}\right\}$$

and (activation energy is in J/kmol and Temp (T_0) is in °C)

$$C_2H_5OH + CH_3CHO \rightleftharpoons CH_3COOC_2H_5 + H_2 \qquad (2)$$

$$r_2 = -k_2 \frac{[\mathrm{C_{acetaldehyde}}]^{1.37}}{[\mathrm{C_{ethanol}}]^{1.67}\,[\mathrm{C_{hydrogen}}]^{0.24}}$$

$$k_2 = 0.11 \exp\left\{-\frac{100902}{R}\left(\frac{1}{T} - \frac{1}{22}\right.\right.$$

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In today's lecture we shall perform a case study on synthesis of acetaldehyde from ethanol. The problem statement is like this acetaldehyde needs to be synthesized from 400 kmol/hr of ethanol flow rate at 60 ^{0}C and 5 atmosphere pressure through an isothermal plug flow reactor of length 7 meter and diameter 11.5 centimeter, the reactor will operate at 8 bar pressure and 275 ^{0}C Temperature.

And this will be governed by the following vapour phase equilibrium power lock reaction kinetics, ethanol will convert into acetaldehyde and hydrogen where the reaction rate is given by minus of k1 into the concentration of ethanol, where k1 is given by this expression, this is the k0, this is the activation energy, R is the universal gas constant and T obviously is temperature in Kelvin.

Now this activation energy is in J/kmol and temperature T_0 which is used in this particular rate expression that will be in ^{0}C. This is about second reaction where we have ethanol which will react with acetaldehyde which is actually the produce of this particular plant and it will produce the ethyl acetate and hydrogen. And the rate expression r2 is this where k2 is given by this expression.

This is k_0, this is the activation energy and this is the T_0 which is in ^{0}C. Now obviously here if you use 1 by T in Kelvin then you really cannot directly write it as 220, you have to write it as 220 + 273.15. So, instead of 220 you have to write this, but just that we want to enter this value in aspen plus simulation window in terms of ^{0}C, so I have just written here as 220 but do not do this mistake while you do the simulation yourself for practice purpose.

And here also the reaction rate depends not only on ethanol but it will depend upon the concentration of acetaldehyde, concentration of hydrogen as well as concentration of ethanol. But one thing that you might understand that this reaction is favourable because it is producing the acetaldehyde which is actually the purpose of this reactor, but this reaction is not desirable.

So, we have to do some operation by which the effect of this reaction is reduced, the feed is initially at 60 ^{0}C 5.5 atmosphere pressure, but the reactor operates at 8 bar pressure and 275 ^{0}C so we need a pump and a heater which will take the feed at this condition before we can feed it into the reactor.

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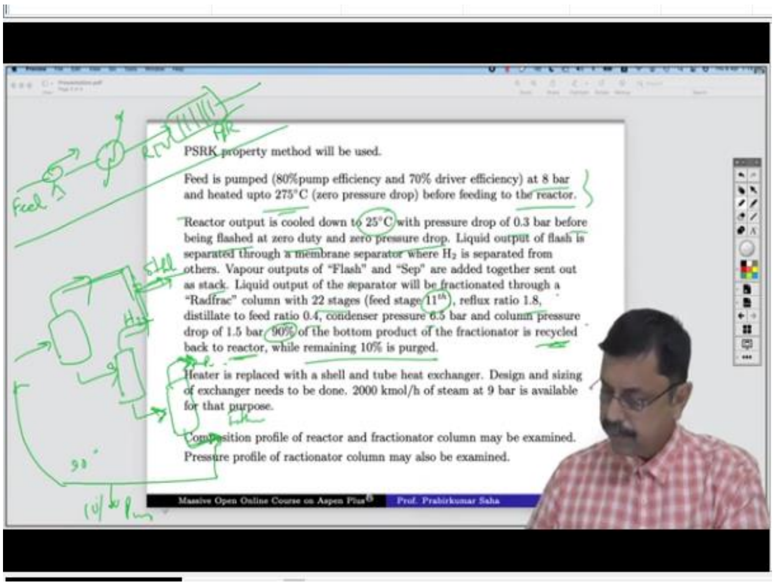

PSRK property method will be used.

Feed is pumped (80%pump efficiency and 70% driver efficiency) at 8 bar and heated upto 275°C (zero pressure drop) before feeding to the reactor.

Reactor output is cooled down to 25°C with pressure drop of 0.3 bar before being flashed at zero duty and zero pressure drop. Liquid output of flash is separated through a membrane separator where H_2 is separated from others. Vapour outputs of "Flash" and "Sep" are added together sent out as stack. Liquid output of the separator will be fractionated through a "Radfrac" column with 22 stages (feed stage 11th), reflux ratio 1.8, distillate to feed ratio 0.4, condenser pressure 6.5 bar and column pressure drop of 1.5 bar. 90% of the bottom product of the fractionator is recycled back to reactor, while remaining 10% is purged.

Heater is replaced with a shell and tube heat exchanger. Design and sizing of exchanger needs to be done. 2000 kmol/h of steam at 9 bar is available for that purpose.

Composition profile of reactor and fractionator column may be examined. Pressure profile of ractionator column may also be examined.

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So, feed is initially pumped at 8 bar pressure and it will be heated up to 275 ^{0}C before feeding into the reactor. So, we will need a pump and then a heater and this one, so this is the raw feed and this will be the reactor input, so here you will have the plug flow reactor. So, this strategy is this one and then reactor output is cooled down to 25 ^{0}C with pressure drop of 0.3 bar before it is being flashed at 0 duty and 0 drop pressure.

So, the reactor output whatever it is will be flashed first and then the liquid output of the flash is separated through a membrane separator. So, we will have a membrane separator like this where hydrogen is separated from others. So, we will have hydrogen at the top and others will be at the bottom. The vapour outlets of flash and separator they are added together so we will add these together and it will be sent out as stack.

So, this portion is understood and what about this outlet? The liquid output of the separator will be fractionated through a Radfrac column. So, we will have a Radfrac column over here the Radfrac column will have 22 stages of which the 5th stage will be the 11th, it will have a reflux ratio of 1.8 and distillate to feed ratio is given, condenser pressure is given, column pressure is given.

Now the 90% of the bottom product of the fractionators, because acetaldehyde will primarily go through the top. So, this is our product and this will primarily contain mostly ethanol and other things until unless we do the simulation we will not know what it is, but mostly it will have ethanol and that needs to be recycled. So, 90% of this bottom product will be recycled back to the reactor while remaining 10% will be purged. So, this one we will split 90% will go to the reactor back as a recycle stream and 10% will be purged. So, this is the complete strategy.

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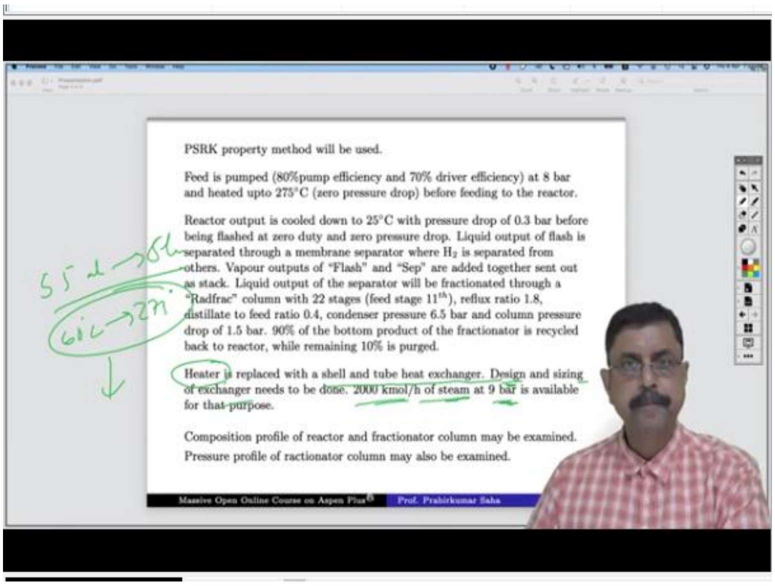

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Now we shall replace the heater with the shell and tube heat exchanger and we will do the design and sizing of the exchanger, for that we have a steam flow rate of 2000 kmol/hr at 9 bar pressure. Now the temperature of the steam has not been given, so we will assume some temperature and check whether that temperature works, if it does not work then we have to give another temperature and check at which temperature it can be operated.

Now composition profile of the reactor and fractionator column may be examined and also the pressure profile of the fractionator column may also be examined. Now let us go to the aspen plus window. Now in aspen plus we shall use PSRK property method that is Predictive Redlich–Kwong Soave property method.

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Now we have to add the components, so what are the components that we have.
We have ethanol, acetaldehyde, hydrogen ethyl acetate, so these 4 components we have, so let us add it ethanol, hydrogen, then we will have acetaldehyde, so just find acetaldehyde, it is a long name so we cannot just write it just like that, so many components but we have to find out the one which exactly we want. So, just go down, this is the one which we want. Similarly, we need ethyl acetate, so just write ethyl acetate, this one.

So, just add it, so we rename them as acetaldehyde and this one you rename as ethyl acetate and finally we add water also, why because we need steam; although it is not working as a process stream but water will be useful for heating purpose because we need steam for heating. So, press next, so the method name will be using predictive SRK, press next, press next again run.

So, it is over, go to simulation so you might remember that we have a strategy that feed will be first passed through the pump and the heater and then finally it will be sent to PFR. So, we will simulate them together. For that let us first add one pump then we will add one exchanger and then we will have a blood flow reactor, in between we will keep a mixer because this mixer will be used to recycle the stream.

In the very beginning mixer will have only one stream later we will add the recycle stream. So, let us keep it as this manner, first rename them, let us write pump, this is mixer 1, this will be heater 1 and this will be PFR. So, we have renamed them just keep it like this heater 1 is over here and this is our PFR. Now add the material stream, this is our original feed, this will come to the mixer.

Then mixer output will go to the heater, heater output will go to the PFR and this is the PFR output. Again, rename them, write it as feed, this is pump output, this is heater 1 in, this is reactor in and this is reactor out. So, we have renamed them, press next. First it will ask for the feed input. So, field input as we know it is 60 ^{0}C 5.5 atmosphere pressure and 400 kmol/hr of ethanol.

So, we write it as 60 ^{0}C 5.5 atmosphere pressure and 400 kmol/hr. of ethanol. So, the feed is pure ethanol. Press next, so it will ask for the heater input, the heater will operate at, so there will be zero pressure drop and 275 ^{0}C is the output. So, it is 275 and zero pressure drop, this is about heater. Then we will have PFR, before PFR let us talk about the pump because PU comes later than PF. So, alphabetically it comes but we will first finish the pump because PFR it has to deal with many more inputs than pump.

So, we have a pump whose discharge pressure has to be 8 bar and its efficiency we know the pump efficiency is 80% and driver efficiency 70%. So, it is 0.8 and this is 0.7, pump is done. Now PFR, we have to feed in lot of information what is the reactor type? Reactor type is isothermal, it is an isothermal PFR, this is an isothermal PFR of length 7 meter and diameter 11.5.

So, go to configuration the length is 7 meter and 11.5 centimeter. So, just write 11.5 over here, press next. So, we have to add reactions, so reaction set r 1 which is of power law type, press next. So, it will ask you to give more details about the power law reaction, press new and then the components. Now check the reactions once again ethanol is converted into acetaldehyde and hydrogen.

So, ethanol is converted to acetaldehyde and hydrogen. So, this is -1, this is +1, this is +1 and exponent. So, just refer to once again k1 C ethanol, so we have exponent of 1 over here, because there is no other concentration which will define this reaction rate and the exponent is 1. So, we have only one exponent that is 1 over here and exponent 0 for acetaldehyde and hydrogen both, because this reaction actually it means k1 C ethanol to the power 1 C of CH_3 CHO to the power 0 and concentration of hydrogen to the power 0.

Now we have to add the second reaction. What is the second reaction? Second reaction is ethanol plus acetaldehyde will form ethyl acetate and hydrogen. So, ethanol plus acetaldehyde will produce ethyl acetate and hydrogen. Here the coefficient is -1, -1 and 1 and 1 over here. What about the exponent? Just check again, here the exponent is 1.37 for acetaldehyde and for ethanol it is -1.67, because ethanol concentration has come down at the denominator.

So, it will be C ethanol of -1.67, for hydrogen is -0.24 and if you take them in the numerator it will be minus. So, for ethanol -1.67, acetaldehyde +1.37 and hydrogen -0.24 and ethyl acetate there will be nothing. So, it necessarily means that the concentration of ethyl acetate does not matter on the reaction rate and that is good news. Why we will learn later? Now let us go to the exponent it is -1.67, acetaldehyde +1.37, hydrogen -0.24 and this one 0 because the concentration of ethyl acetate does not affect the reaction rate.

Now go to the kinetics. The first reaction the k value, so the k value 1.5 10 to the power 9. So, it is 1.5 into 10 to the power 9 and the activation energy is 8.5 into 10 to the power 7 and it is J/kmol. The next reaction k2 is 0.11. So, go to the next reaction, this reaction in the first reaction we did not have T_0 specified. So, we used this but the second reaction we have a T_0 specified.

So, we have to give it in this fashion, look at it in both the cases we have n = 0, n means you look carefully here n is t by T_0 to the power n, so here n is 0 because we do not have anything of this nature. Here also t to the power n but we do not have anything of this nature in our rate expression. So, for us n is always 0, but we have a k which is 0.11. So, write 0.11 here and activation energy it is 100902.

So, just write 100902 and this is in J/kmol and T_0 it is in ^{0}C 220. So, if you add 273 over here just to make this reaction looked at, in that case you have to write 493 Kelvin, you have to write here Kelvin. So, be careful about what information you give over here. Now the kinetic is well defined, now the plant is well defined to run though it is a part of the whole plant anyhow.

So, let us see the stream results now, go to the stream result of the PFR. So, this is the reactor in, this is the reactor out, an isothermal reactor so the temperature does not change, the pressure does not change, the molar flow reactor in it was 400 kmol/hr of ethanol and reactor out is also 400 kmol/ethanol. There is no production of acetaldehyde and hydrogen or ethyl acetate.

There must be something wrong that we have done. So, let us go back and check what wrong we have done. The problem is over here, the reaction input. What did we say about the kinetics? We said the reacting phase is liquid, but is it so? Is the reaction phase liquid just go and check the vapour fraction in all the cases? What is the vapour fraction? Here it is 0, so completely liquid, this is also completely liquid, this is also completely liquid, but after heating it becomes completely vapour.

So, whatever is entering into the PFR that is completely vapour and what is coming out that is also completely vapour, because at temperature and pressure so at 8 bar pressure and 275 ^{0}C the ethanol can never be in liquid phase. So, it will be in completely vapour phase. So, that we have a PFR which is in completely vapour phase. So, while specifying the kinetics we have to say reactor phase vapour.

If we do not give this information it will not work. Second case also it is vapour phase, run the simulation once again and check the stream result of PFR, yes now the molar flow rate has changed that means we have some reaction that has taken place, we have 43.6749 kmol/hr of ethanol is left out. This is unreacted which actually we need to recycle, hydrogen 356, acetaldehyde 110 and ethyl acetate which is undesired product, it is 122.948.

So, this is the reactor output. Now we will do the recycle later, but before that we have to do certain operations. First thing first we have 43.6749 kmol/hr unreacted ethanol that means the ethanol has not been fully converted, why because the size of the reactor volume is not enough. So, if we change the configuration instead of 11.5 centimeter let us use 15 centimeters.

So, we are taking a larger diameter PFR, what happens then, let us run it once again and check the stream results, you will find the entire ethanol has been converted into the products. That means by tweaking the configuration of the PFR you can negotiate with the extent of reaction and extent of conversion of reactants. Any way we will not go into that because we have to learn how the recycle works.

So, for that let us go back to our original configuration, it was 11.5-centimeter diameter. Let us run and check the stream results and we get the 43.67 kmol/hr of unreacted ethanol and we have to work with that fine. So, we are standing over here. Now what we need to do? Just go back a few slides this side here. So, the reactor outlet has to pass through a flash tank in series with a separator, in series with a radfrac.

So, the vapour outlets of flash and separator they will be added and sent out as a stack. The liquid outlet of separator will be sent into the radfrac where they will be separated as vapour and liquid; we will see what they have. So, we have to place a flash over here then a separator and finally one radfrac column. So, first rename them, so we have flash, this is a membrane separator and this is fractionated.

Just put it on them, do not need to clutter. So, add this one like this, then material this one gets connected with this, this one goes like this, this one connected with this, the upper one goes like this, we will add them together let us simulate first and check what they are and then we will add this is the top product of fractionator, this is the bottom product of fractionator.

This will mainly be acetaldehyde which is the product and this stream we will recycle, but before that let us rename them. We will call it F-vap, this is F liq, this is M-vap, this is M-liq, this is fractionator vap and if vap already exists because we have used F for flash. Here we can write C vap column vapour and this is column liquid. Now they will ask for the details of flash membrane and fractionator.

So, let us check, before that we have to cool down the reactor output to 25 ^{0}C and 0.3 bar pressure. So, before flash we have to insert 1 cooler. So, for that we select this insert block ID cooler 1, say eater model, temperature 25 ^{0}C and pressure -0.3 bar. So, there is a pressure drop of 0.3 bar, 25 ^{0}C and pressure drop 0.3 bar. So, the heater is done, so we will rename it, first we will write it as F-in and this one will write R-out, now it will ask for flash and membrane.

So, for flash it will be flashed at zero duty and zero pressure drop. So, press next, so it is zero duty and zero pressure drop, next is fractionator. Let us first define the membrane separator. In the membrane separator we take the strategy to employ such a membrane which separates hydrogen from all other components and send it through the top. The remaining components whatever they are come through the bottom of the separator. So, only hydrogen goes through the M-vap.

So, we check M-vap and we write split fraction of hydrogen is 100%, all others are 0. So, membrane separator is defined, the last is the fractionator. So, fractionator is equilibrium time, number of stages, 22 stage, free stage 11, reflux ratio 1.8. So, 22 stages condenser is total; we do not know distillate rate but we know the distillate to feed ratio which is 0.4 and reflex ratio is 1.8.

Go to streams the feed stage is 11th and the condenser pressure it says 6.5 bar and the column pressure drop 1.5 bar. So, it is 6.5 bar and column pressure drop are 1.5 bar that means condenser pressure is 6.5 and column pressure drop 1.5 means the reboiler pressure or the bottom product output will be 6.5 + 1.5 that is 8 bar pressure which is equal to the reactor pressure.

So, definitely we can recycle it, so now it is ready to run, so run it, so just check what is the F-vap content? We have 3 for 55 kmol/hr of hydrogen, only 1.2 ethanol, 22.25 acetaldehyde and ethyl acetate are 3.47 kmol. So, in terms of mass flow or say mole fraction we have 92.96% of hydrogen almost pure hydrogen, very little amount of ethanol and ethyl acetate to some extent acetaldehyde.

So, this is basically hydrogen stream and we have the membrane separator which is throwing out hydrogen through M-vap where we have 0.644505 of kmol/hr of hydrogen, all others are 0. So, we are adding them for that we have to add one mixer. So, we just add the mixer over here and let us rotate it once here. So, let us add it like this and add it over here. Yes, so this is mix 2 and the output of mix 2 is so we write it as M2 out.

Now it is ready to run, yes now check about amount, we have 356.325 hydrogen with a mole fraction of 92.97. So, now let us see what is the outlet of C-vap and C-liquid. For that let us open fractionator and stream profile of the fractionator. Here you see we have 87.8163 kmol/hr of acetaldehyde that is going through vapour phase, no hydrogen little amount of ethanol and little amount of ethyl acetate.

While most of the ethanol is going through the liquid phase where we do not have acetaldehyde and ethyl acetate. So, let us freeze this figure for later use. Now before recycling you notice one thing. If you go and check the reactions once again you can see over here this is the desired reaction, this is undesired reaction. Concentration of ethanol favors the desired reaction and it does not favour the undesired reaction.

Because if we increase the concentration of ethanol then the reaction rate decreases for the undesired reaction. So, it is good for us to increase the ethanol concentration. So, recycle of ethanol rich stream will be favourable for our system. Now in the bargain we are recycling acetaldehyde also, concentration of acetaldehyde favors the undesired reaction which is not good, we do not want that.

But then check the stream once again, the stream result. Here you see the concentration of acetaldehyde is very small, compared to that concentration of ethanol is high. That is exactly what we want. So, here we are not doing the recycle just for the sake of it, we are doing the recycle with a proper thinking and if the reaction is favoured by the recycling then only we will do it, it might so happen that the concentration of acetaldehyde will be very high or it may be saying 50% and 50% of both.

In such situation the reaction might not favour because you can check it is 1.3, it is 1.67. So, marginally it will favour but mostly it will not favour because if the concentration of acetaldehyde is more in that case more and more amount of ethyl acetate will be produced which will be waste for us. So, the takeaway from this exercise is we are not doing the recycling just for the sake of it we have to do the recycling after proper thinking.

And if only the desired reaction is favoured an undesired reaction is not favoured by recycling then only will do otherwise we would not do. So, let us go back to the simulation, we have to do the recycling but before that we have to split it because 90% of the bottom product of the fractionator is recycled back to the reactor while remaining 10% is purged. So, let us use a splitter.

So, this is a splitter, we will rotate the icon, so connect this thing with this; then connect this with this and then this is another product which is purged. So, few cosmetic changes, so we write it as recycle and we rename it as purge. Now press next, so the split what is the split fraction of purge? It is 10%. So, write 0.1 and it is ready to run, so the 90% will go to recycle. So, run is complete. Now check what is the evaporator concentration.

So, this is the only product right now, all other we have recycled. So, 226 kmol/hr of acetaldehyde is coming out from the top while 50 kmol/hr methanol is going out through the same stream, ethyl acetate which is waste product it is very small amount. Earlier we had this information you just check. So, this is without recycling, we had in C liquid or C-vap you can check acetaldehyde was only 87.81.

But now it has jumped from 87 to 226 nearly 3 times jump in the acetaldehyde production just by using the recycle stream which is good. So, we have done up to this point, now we have to replace the heater with a shell and tube heat exchanger and its design and sizing needs to be done. We have 2000 kmol/hr of steam at 9 bar pressure. Before that let us see how much of heat duty it is having.

This heater we have to replace and this heater has a heat duty of 2780262 heat duty. So, we note down this number 2780262 calorie per second because this is the unit that we are using, press a heater over here, attach material stream and rename it as steam in and this is steam out and this heater duty is same as this one in the negative way because h 1 is heating the fluid from 103 to 275 ^{0}C.

And its duty is 278 0262 cal/sec, we shall be using a heat exchanger that will use the steam for that heating purpose, we are aware that cooling at the rate of 2780262 cal/sec will be carried out at the steam side we want to know the outlet condition of the steam. So, for that let us use a heat duty of 278 it will be minus because it is a cooling 2780262 with zero bar pressure drop. So, press next.

The steam input, we do not know the temperature of the steam, let us use 300 ^{0}C. Steam is available at 9 bar pressure and 2000 kmol/hr of flow rate it has, now it is ready to run. So, run it, so we have got the information it is -2780262, its temperature is 175 ^{0}C and it is not completely steam 56% is vapour fraction and rest is liquid fraction.

So, it is mixture of vapour and liquid this end. So, now we replace, so first we have to cut it and we have to place a heat exchanger. So, attach it as cold stream, attach it as cold output and this one you have to reconnect the stream, so reconnect this stream with this destination and reconnect this stream with this source. So, basically, we have done a parallel calculation of the heater and after the calculation is over we are attaching them with the main calculation that we need.

So, there is no purpose of this heater now so we can simply cut it. So, rename it as heat exchanger, write it as heat ex no problem and press next, it will ask for the details of heat exchanger. Now let us use shortcut heat exchanger calculation in the very beginning, so it is shortcut heat exchanger with a specification of heat duty which is 2780262, the same as the heater and run it and check whether initially it will work or not.

Now it says that there is no problem all of them it has run beautifully. So, it is likely to work, but we have to go further into it. Let us check the T q curve and see whether the temperature profile is acceptable.

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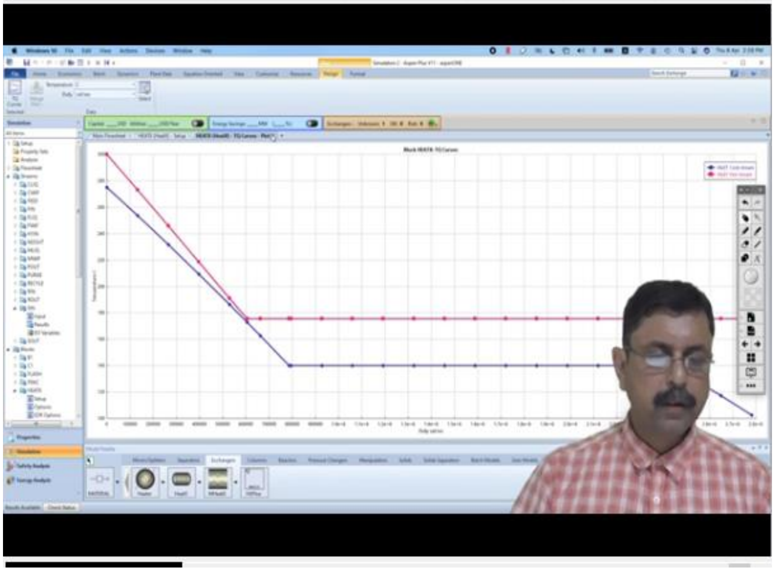

Now we have a temperature profile and we find that there is narrow difference between the cold stream and hot stream at this point. So, this we do not like, so our idea is to have a wider gap between the temperatures of cold stream and hot stream, otherwise there can be a failure in the run.

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So, for that we have to change the stream temperature, so we have assumed 300 in the past. Let us use 350 instead and check what happens, run once again and go to the heat x block check the T q curve once again, now it is fine, we are happy with this. So, we change from shortcut to shell and tube heat exchanger. So, when we click it, it is asking us to convert to rigorous exchanger. So, it is asking to select the exchanger type which is shell and tube, select conversion method size exchanger or specify exchanger geometry.

Now if we have the exchanger geometry with us we can feed in the data, otherwise let aspen calculate the best possible geometry for this type of exchanger, so, press convert. So, here it has opened a console EDR sizing console. Now in the process stream you may change everything to a unit with which you are comfortable, the pressures we have changed to bar, temperature in ^{0}C, heat exchange in say megawatt and fouling resistance in SI unit.

And geometry; the various types of configuration B is for bonnet bolted integral with tube sheet, there are so many types you can choose one of them, E means 1 shell pass, 2 shell passes with long baffles, split flow, double split flow etcetera, keep it default, M is again bonnet integral channel with flat cover, there is various options. An experienced designer always can play around with this kind of choices because their experience they know what kind of demo type will be most suitable for their need.

But for a learner there is no point in going into these details let us keep it with the default values. Location of hot fluid in the shell side tube OD and pitch if you want to change it you change otherwise you keep it default, tube pattern whether it is 30 ^{0}triangular, rotated triangular square, rotated square, you can choose the tubes in baffle window or not baffle type whether it is signal or double segmental, triple segmental etcetera.

Baffle cut orientation whether it is horizontal or vertical and so on. Size specify some sizes for design, if you have certain information something like shell ID. Suppose you have a space constraint and you do not want your shell ID to be calculated beyond the space that you can give it for that kind of shell. So, you can say that shell ID is this much of inches. So, aspen will know that you have the space constraint.

And aspen will calculate all other parameters to fit in within that shell ID. Similarly tube length if you do not have any constant of tube length just leave it otherwise you can give some information that my tube length should not be more than this size. Otherwise, you will not be able to fit in to that particular designated place for your exchange. If you do not have any constraint of that nature just keep it no let aspen calculate.

So, press size and it is doing EDR sizing or optimizing. So, it has evaluated so many designs and they are finding 30 designs are very near. So, it will take some time; let us wait patiently. So, evaluation is completed and it is giving us the setting plan if you want to know the tube layout, so this is the suggestion of tube layout, you can check what is the tube layout like this and they have calculated the shell ID to be 53.1496.

Now it is an odd figure, so what you can do you can write it as say 55-inch, tube length 236 you can write 240 and baffle facing 24 say, so it will be 10 baffles and if you have some more information like this you can just give or just leave it as it is and press accept design. So, this design is now accepted. Now you have to run it once again for the simulation. So, the simulation is done and unfortunately there is some error messages coming let us see what kind of error message it is.

There is an error message in thermal results, just check what is the status, so it is not error, it is a warning a possible vibration problem has been identified now. Vibration problem is a mechanical problem, so it is not a process engineering problem, as a chemical engineer you do not have to worry about it. The mechanical engineers who will actually design the mechanical details they will try to figure out how to deal with it.

But as a process engineer, as a chemical engineer you have to check whether this is possible or not and it is yes, it is possible the block calculations were completed with warning that we know and property calculations were completed normally. So, as a chemical engineer you should be happy that property calculations and process calculations are done and if you want to see the stream results you just go and check.

So, this is the stream result. Now one thing that you can see that if you change it to 350 ^{0}C then the temperature is 303, the inlet and outlet temperature the isothermal reactor now it is working at 303 ^{0}C instead of 275 ^{0}C and we are not happy with this. Now if we change the temperature from 350 to say 340 then let us see whether any difference we get yes.

So, let us see the results, at main floor sheet, now it has come down to 298. So, perhaps we have to go further down in order to make it 275 ^{0}C. Now let us check some more things over here what is the reactor concentration profile? For that just press the concentration profile or composition profile and press ok.

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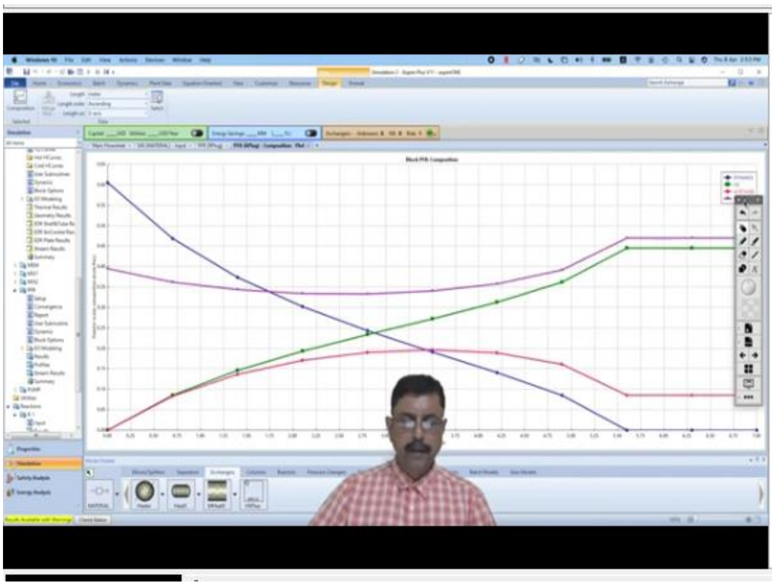

So, here this one is ethanol line which is continuously decreasing. Hydrogen is continuously increasing, acetaldehyde is going higher and then after some time the recycling is occurring so it is going down and finally it should be ethyl acetate. So, here it says that 5.6 meter is sufficient for entire reaction to be over. Now actually it should use the total length 7 meter but it is using only 5.5 meter or 5.6 meter.

You see the ethanol is becoming 0 at this point.

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This is because by changing this flow rate we are changing the temperature also. So, the reactor is now operating at higher than 275 ^{0}C. So, somehow, we have to lower down this temperature. So, we have to manipulate the heat x to some extent, whereby the reactor input temperature remains at 275 ^{0}C, it should not go beyond that. Now go to fractionator and check the composition profile, so both vapour and liquid, select all.

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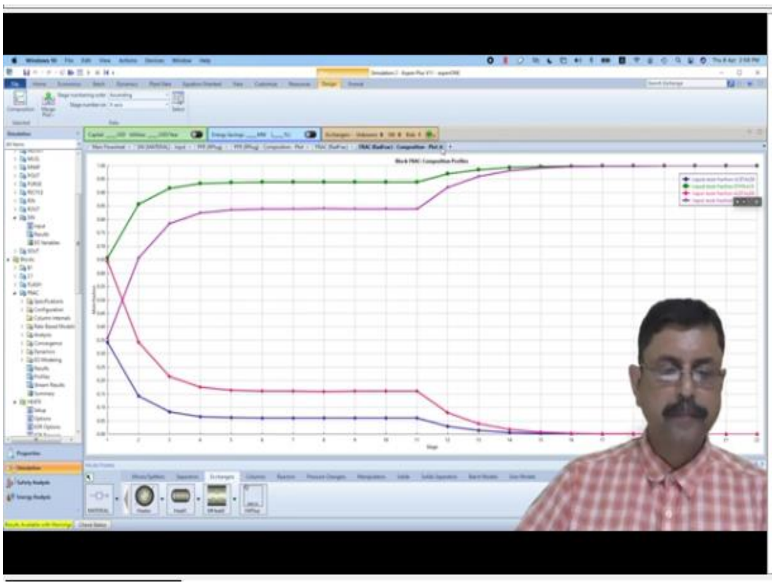

So this is the fractionator, we have acetaldehyde and ethyl acetate. Hydrogen completely has gone off and we do not have any ethanol left, so there is no profile for ethanol over here, because of the change.

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Now if we want to see the pressure profile very straightforward it should be a straight line.

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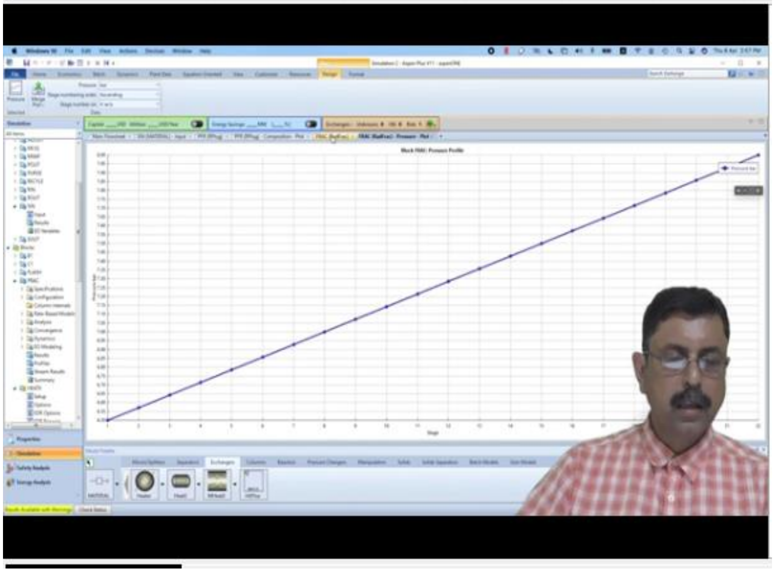

Because it is a straight line starting from 6.5 to 8 bar pressure at 22 is stage is the re-boiler. And then you can check the k value profile, relative velocity profile, flow ratio profile etcetera, whichever profile you want to check just press that particular icon you will get the profile.

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So, with that we come to the end of this case study, we will continue in the next lecture with another case study, thank you.