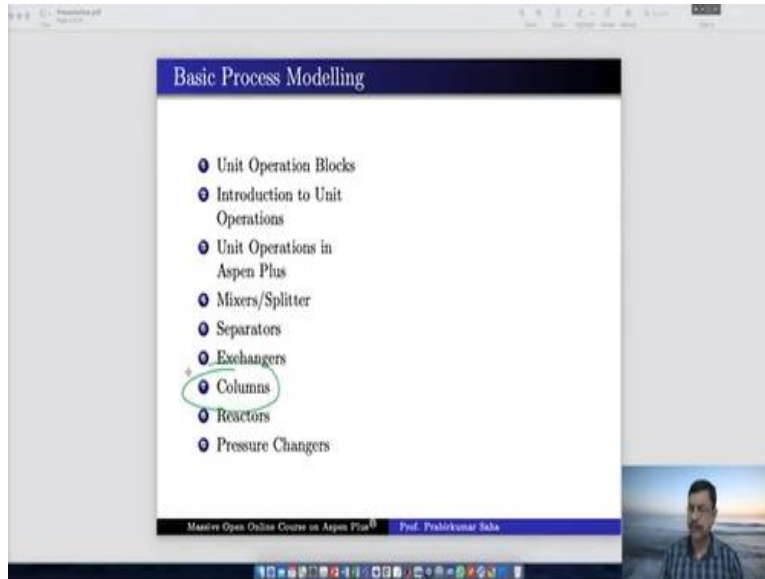


Aspen Plus Simulation Software - a Basic Course for Beginners
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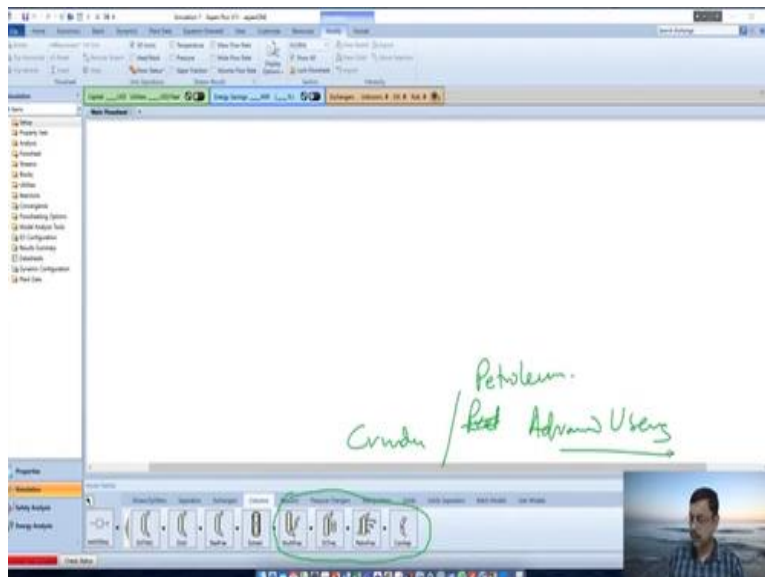
Lecture - 06
Using Model Pallete - Columns

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Welcome to the massive open online course on Aspen plus. To continue with this lecture series on basic process modelling. Today we will discuss about the columns.

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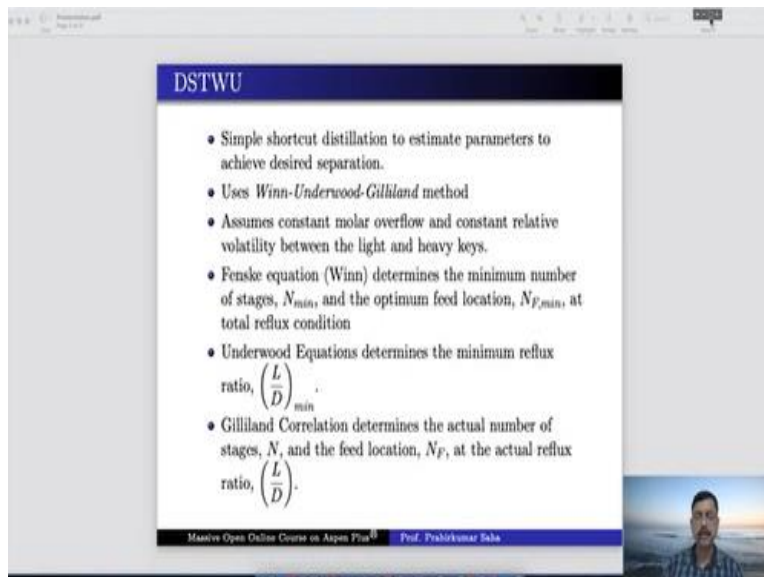


If you look at the Aspen plus simulation window you will find various types of columns to operate DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac and concept. We will go one by one. DSTWU, it says it is shortcut distillation design using the Winn-Underwood-Gilliland method. The second one is distl, again it is shortcut distillation rating using the administer method.

Third one is RadFrac, it is used for rigorous two or three phase fractionation for single columns it can model absorber stripper etcetera. Extract model it is for rigorous counter current extraction of a liquid with a solvent. It can model liquid-liquid extractor. And we have four more the first one is rigorous fractionation for complex columns such as crude units. The second one is shortcut distillation for complex columns such as crude units and vacuum towers.

The third one is Petro frac that is rigorous fractionation for petroleum refining applications such as pre-flash towers and finally it is concept it performs feasibility and design calculations for distillation column. So, you can understand that these four are mainly for crude and they are principally used in petroleum industries. Obviously, they are for advanced users and they are not within the scope of discussion in this lecture series. So, in today's lecture we will limit ourselves within the first four that is DSTWU, Distl, RadFrac and Extract.

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The image shows a presentation slide titled "DSTWU" with a list of bullet points. The slide is displayed in a window with a standard Windows-style title bar. In the bottom right corner of the slide, there is a small video inset showing a man speaking. The slide content is as follows:

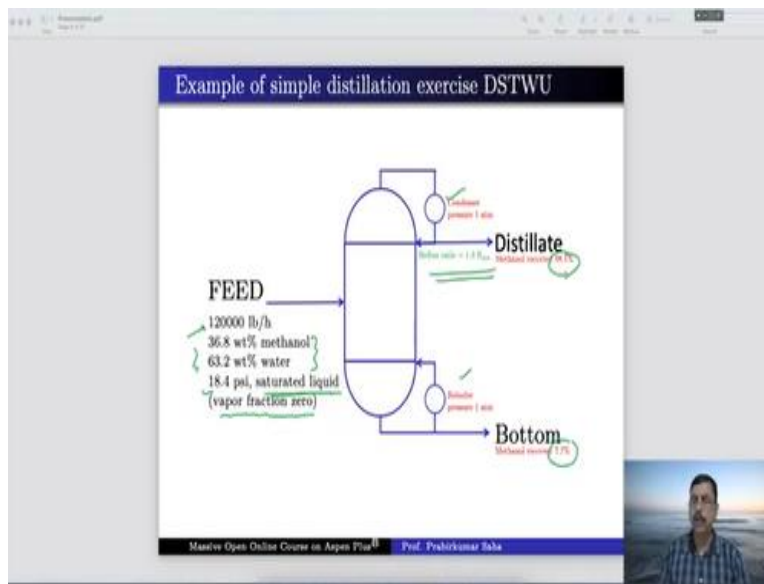
- Simple shortcut distillation to estimate parameters to achieve desired separation.
- Uses Winn-Underwood-Gilliland method
- Assumes constant molar overflow and constant relative volatility between the light and heavy keys.
- Fenske equation (Winn) determines the minimum number of stages, N_{min} , and the optimum feed location, $N_{F,min}$, at total reflux condition
- Underwood Equations determines the minimum reflux ratio, $\left(\frac{L}{D}\right)_{min}$.
- Gilliland Correlation determines the actual number of stages, N , and the feed location, N_F , at the actual reflux ratio, $\left(\frac{L}{D}\right)$.

At the bottom of the slide, there is a footer that reads "Masive Open Online Course on Aspen Plus® Prof. Prabhakar Saha".

First, we begin with DSTWU as there is simple shortcut distillation to estimate parameters to achieve desired separation. It uses Winn-Underwood-Gilliland method. It takes two assumptions one is constant molar overflow another is constant relative volatility between the light and heavy keys. Now Winn that is the Fenske equation it determines the minimum number of stages and the optimum feed location at total reflux condition.

Whereas Underwood equations they determine the minimum reflux ratio and the Gilliland correlation that determines the actual number of stages and the feed location at actual reflux ratio. So, we shall learn the DSTWU block and its efficacy with the following example.

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So, this is the example of simple distillation exercise. So, this is a column the feed contains a mixture of methanol water its flow rate the weight fractions pressure they are given and also it is said that feed is saturated liquid. Temperature is not given but it is said saturated liquid that means the vapour fraction is 0. So, this information is needed for the simulation purpose. The distillate contains 98.1% of methanol whereas the bottom product contains 7.7% of methanol.

Both condenser and reboiler they operate at one atmosphere pressure the reflux ratio is 1.3 times of the minimum reflux ratio. So, with this information we will use the shortcut distillation method using Winn-Underwood and Gilliland method. So, let us go to the simulation window.

(Video Starts: 03:59)

First, we have to go to the properties and we have to enter the components methanol and water. Press next we shall use the NRTL-rk method which is nrtl renon with Redlich-Kwong equation of state with Henry's law. We will use this because for methanol water system this is the best property method that we can have. Press next run go to simulation window go to column take this DSTWU connect the material streams rename them write it as feed write it as DS DIST for the DSTWU DS BOTT.

We are using these prefix ds because we are going to use the distillation RadFrac also and compare. Press next last for input for feed material so we have the information it is at 18.4 psi and vapour fraction 0, the feed rate is 12000 pounds/hour mass flow rate. So, we are using English unit. So, convert it in 12000 mass fractions, methanol is 36.88% and water is 63.28%. So, first one is 0.368 and then 0.632. 0.368, 0.632 so total it comes 1, we have to change it to mass fraction.

Press next, here it is asking for the inputs for the block b1 running with DSTWU. So, you can either specify number of stage or you can specify reflux ratio. Now we have the information of reflux ratio not the actual reflux ratio but we know that reflux ratio is 1.3 times of the minimum reflux ratio. Here in the reflux ratio if we write 1.3 then the actual reflux ratio will be taken as 1.3. But if we write -1.3 then minus indicates that we are referring to 1.3 times of the minimum reflux ratio.

So, that is what the prefix minus means over here, it is not negative sign it is 1.3 times of the minimum reflex ratio that is what it means. The condenser and reboiler both of them operate at one atmosphere pressure. So, for both of them we write 1 and 1, the light key component obviously it is methanol and recovery is 98.1% so, we write here 0.981. The heavy key is obviously water and here the methanol recovery is 7.7% so it is 0.077 so here it is 0.077.

So, the specifications are complete now it is ready to run. Let us run the results are available let us see the results first. So, here the minimum reflux ratio has been calculated as 0.607989. So, this is system calculated minimum reflux ratio. Here the actual reflux ratio is 1.3 times of the

minimum reflux ratio. So, if you multiply this with 1.3 then you will definitely get 0.79385. Minimum number of stages is 4.62 and the actual number of stages is 9.

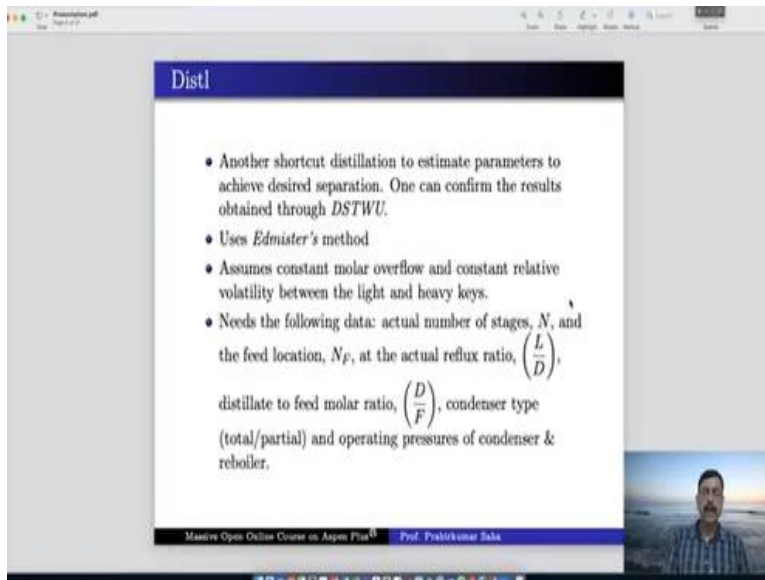
Actually, it is saying 9.00 because it is calculating that way in reality number of stages cannot be fraction so we should take 9. Feed stage is 5.47768 now here also we have to take 5 for actual operation. Reboiler heating required is in British thermal unit it is given in Btu by etcher. But we can change this unit to say megawatt it is 14.026 megawatt of duty is required for this reboiler and condenser cooling required also is around the same 13.8302.

Distillate temperature and bottom temperature both are given. The bottom temperature obviously it should be near to water boiling point. And here another important information is distillate to feed fraction it is almost 0.3. This information will also be required in future calculation. Now let us see the stream results, so these are the stream results this is bottom product and this is distillate product here you can see the total mass flow rate is 1200 in the distillate we have 49160 rest is going at the bottom.

Now the methanol content is 43321 in the distillate only 839 goes to bottom. Whereas water out of 75840 pounds/hour 70000 goes to bottom only 5839 goes at the top. So, this information will be required for us in further calculation.

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The next one is Distl. It is another shortcut distillation to estimate the parameters to achieve desired separation and one can confirm the results obtained through DSTWU. It uses the Edmister's method and it also assumes the constant molar overflow and constant relative volatility between the light and heavy keys. And to operate it needs this following data it needs actual number of stages the feed location the actual reflux ratio and the distillate to feed molar ratio.

It also needs the condenser type whether it is total or partial and it also needs the operating pressure of condenser and reboiler. So, all this information we already have from our previous calculation of DSTWU. So, now we will solve the same simulation problem using Distl not with DSTWU. But we will not delete the DSTWU simulation because we need this information in our next simulation.

(Video Starts: 10:01)

So, let us go to our next simulation. For that let us go to main flow sheet. Here we do not delete that the previous simulation we will just copy now we do not want to delete this part because we need it, we just make some cosmetic changes over here. Here we rename it as Distl distil block. Now we will use a manipulator over here this is a duplicator. So, this duplicated block it just duplicates the streams as if the same stream is going in two different paths.

So, for that we have to connect with this and then material feed to this one material feed to this one again outlet and outlet. So, we rename it as DI-DIST and this one is DI-BOTT. Then we put next obviously the feed information has already been given it is just duplicated now we have to give the information on the distil block. So, here in the distil block we need to give the number of stages.

So, the number of stages already we have this information over here, so number of stages is 9. So, we just give this information 9 and remember we have to give a whole figure we cannot give 9.04 because it is actual number of stages. Feed stage same information is their feed stage is at 5.47. So, we will give 5, reflux ratio 0.790385 this led to feed molar ratio 0.299958. So, we can write it 0.3 not a problem condenser type is total pressure again it is one atmosphere one atmosphere we run it so our results are available.

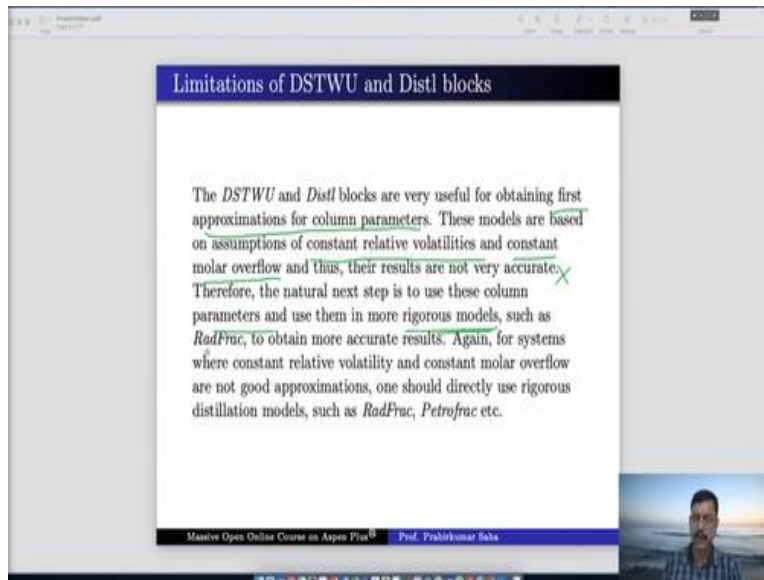
Now we will see this result check the condenser duty first in megawatt it is 13.831 slightly lower than the previous one and reboiler is 4.0285. Earlier we had 14.026 and here we have 14.0285 almost same. Now obviously we are interested to know the stream result. So, let us write here DS-DIST in place of DI, DS-DIST we will write DI-BOTT over here. So, the bottom product of DSTWU block and Distl block they are written side by side;

The same arrangement can be done for distillate also so that we can compare it better. Here again we see the slight difference between the methanol production in the distillate using Distl the quantity is slightly higher.

(Video Ends: 12:56)

Obviously here we are not actually in ideal condition we are doing it in the real condition. In DSTWU block we used the information in fraction form the number of stages was fraction the feed stage was fraction but here it is actual, so it is 9 it is a whole figure 9, 5 etcetera. So, the final result will be slightly different.

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Now we will understand the limitations of DSTWU and Distl blocks. Both these blocks are very useful for obtaining first approximation of the column parameters, because these models are based on assumptions of constant relative volatilities and constant molar overflow so, thus their results are not very accurate. Therefore, the next natural step is to use these column parameters and use them in more rigorous mode.

And what is the more rigorous model? We have RadFrac. So, the next thing that we are going to do is using RadFrac model to solve this problem.

(Video Starts: 14:00)

We have to use now the RadFrac model and compare with the previous two. So, for that we again go back to main flow sheet pull it down over here this RadFrac connect the material streams this is outlet distillate this is bottom write it as RadFrac dist and RadFrac Bott. Press next it will ask for the column parameters, here the calculation type it is suggesting equilibrium. Now two types of calculations we can do equilibrium and rad based.

We will do one by one, for this calculation we will use only equilibrium model but later we will see the rad based calculation for some other problem. Number of stages we have to give 9, condenser is obviously it is total condenser no vapour fraction. Reboiler we can use either kettle

type or thermosyphon type let us keep it as kettle type and we have to give this operating specification either of two.

So, we have display trade, bottom straight reflux rate, boil up rate, boil up ratio and others. Let us use distillate to feed ratio because this information we already have from our shortcut calculation. So, distilled to feed fraction is 0.3 so we will use this information over here 0.3 and reflux ratio that also we know it is 0.790385. So, here all the information that we; have got from shortcut distillation.

So, shortcut distillation block is very useful for giving you the first approximation of this we can fine tune it later. Streams the feed stream the location of feed stream we know it is stage number 5 on stage number 5 so not above it is on stage number 5. Then you have to give the pressure obviously the condenser pressure it is asking for condenser pressure which is one atmosphere we already know it from our problem. So, the simulation is ready to run.

Here the stage two pressure and stage pressure drop their optional information you can give if you have the information even if you do not have no problem the simulation can run either way. So, now you can run the simulation, simulation results are available. So, let us see the simulation results here you can see heat duty in watt let us use megawatt it is better the condenser is 13.8491-megawatt DSTU shortcut it was calculating as 13.83 this is calculating as 13.84 almost same.

The same thing will be they are for reboiler also heat duty is 14.04. Now we are interested to know the stream results. So, here we will take RadFrac bottom here we take DS-DIST then DI-DIST and here we will say RA-DIST. Again, you check the mass flow rate methanol 0.015717 all of them are same. Slight difference will be there because one is rigorous calculation another is shortcut calculation these differences will be inevitable.

Now this can do much more rigorous calculation because you can design the column internals till now, we were not doing any mechanical design of column internals but with RadFrac we can definitely do it. Let us say how? Here you have the option for column internals. So, you can add

column internal generate, so here you have the internal. So, a pictorial form of column is demonstrated starting from stage number 2 to 8 because we have 9 stages stage number 1 is condenser stage number 9 is reboiler.

So, rest of the stages are from 2 to 8 the feed stage is 5. Now we have to add a new section you can design the upper section and lower section separately or you can design them together. Let us design them together. We can we should not complicate the matter so we will say add new. So, this is the section number 1 we start at stage 2 and end with stage 8. Now here we have the option of interactive sizing as well as rating.

The beauty of interactive sizing is if you give very little information Aspen plus based on its inbuilt data and information it can calculate and suggest you some column internals and those column internals can be suggested and viewed by pressing this detail. Now internal type it is tray it can be tray or it can be packed for the time being let us choose tray only. Tray type it can be sieve it can be bubble cap and lot many other types are there for the time being let us choose sieve.

Tray spacing and diameter it is suggesting the Aspen plus is suggesting this dimension if you view the internals more it will give you further information that is what is the whole area if this is the sieve then whole area/active area is 0.1 you can choose number of holes also. What is the side down cover width? Top and bottom sidewall length wear height down cover clearance diameter tray spacing everything is being suggested by Aspen plus itself.

You do not have to give any information Aspen plus can do the simulation with this later if you are not happy with the final result you can do the fine tuning over here. But let us assume that these are correct and you are happy with this let us run the simulation. So, the simulation results are available, so these are the column hydraulics it says that total height is 4.26 meter. So, column height total head loss this much total pressure drop number of trays/pack stages is 7 all these information total residence time everything is given over here.

And column internals you can again view it and you will find the tray type press spacing and the limiting condition of all of them. Now this limiting condition is very, very important and you can further scrutinize them by seeing this hydraulic plot, it is very important. If you go and check the hydraulic plot you will find that not all the trays are good the tray condition is pictorially given by this.

Now here if you see say fourth fifth tray this is the constant v by l line and operating point is over here. So, this is the area where your operating point should lie at each and every stage. It should not go higher than that because this is the maximum entrainment line. It should not go beyond this because it is weeping line this is 100% weeping dumping line this is the minimum wire load this is maximum wire load.

So, all these are written over here what is what those lines they mean each and everything is written so you can go through them. Now here we can understand that stage number 5 to 8 they are good but 2, 3, 4 they are not good. So, we find a cross mark over here. So, what we will do? We will go and check what is the problem? The problem is in this tray say number 2 the operating point is over the maximum entrainment.

So, there is a condition of flooding over there so we have to reduce the flooding. So, the best way of reducing the flooding is to increase the diameter. So, let us increase the diameter of the column. So, go back to geometry here we have the diameter so let us use 3 meter and see what happens? Let us run the simulation once again with this diameter so run is complete. Now we go back to column hydraulics once again now it is fine.

The entire column is blue earlier the top portion was red now each and every point. So, this is the tray number two which is coming within this three also is coming within this 2, 3, 4, 5, 6, 7 everything is within the limit of entrainment. So, the column is running fine. So, here we see starting from 2, 3, 4 earlier we saw a cross mark for first three trays. Now the cross mark has gone because the operating point has come down from here to here.

So, like that you can check the hydraulics and other matters. In this section we assume tray column instead we can use pack columns. Now if you assume packed column then we have to see the packed height also. What is the section packed height? Let us say we will use 5 meter of packing and check whether our simulation runs good so run it. The simulation has run, let us go back to see the hydraulic plot, yes.

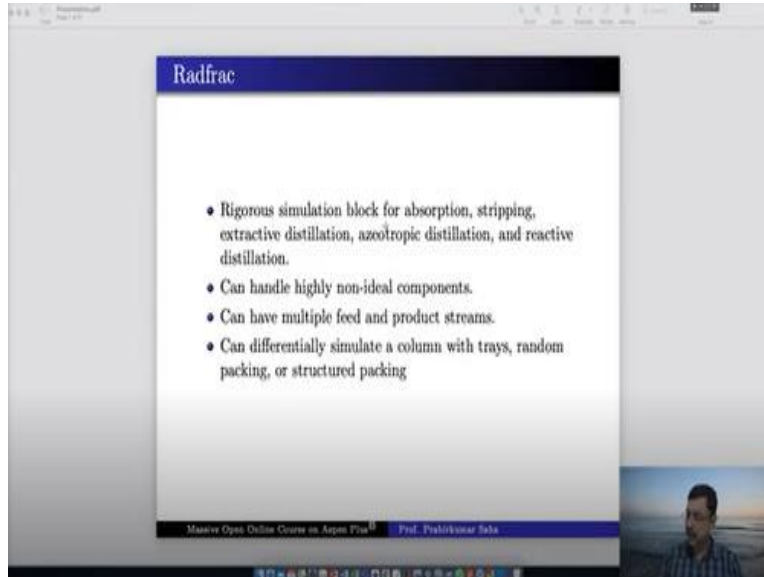
So, the operating point is within the limit so, this is the minimum liquid rate and this is the so here it is minimum pressure drop/unit pack height the dotted line. So, it is way above the minimum pressure drop and this line is allowable pressure drop/unit packed height so, it is way below that and this is the minimum liquid rate. So, that is also met from the very first tray so 2, 3, 4 all the trays they are meeting the criteria.

So, this is how you can do the design of packing. Now the packing material also you can check here the packing characteristics we are using generic model. We can use Raschig green with ceramic material dimension we can check the packing size also we can check and many other parameters we can change and rerun the calculation to see what is the final output.

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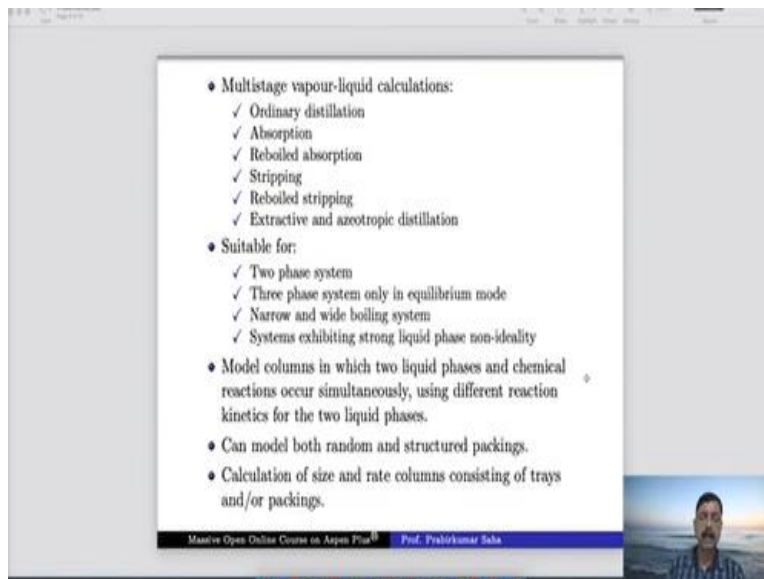
So, that is how you can do the simulation with RadFrac and that can be rigorous calculation. Now we can summarize the features of RadFrac block.

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It is a rigorous simulation block for absorption, stripping, extractive distillation, azeotropic distillation and reactive distillation. It can handle highly non-ideal components it can have multiple feed and product streams it can differentially simulate a column with trays random packing, structure packing.

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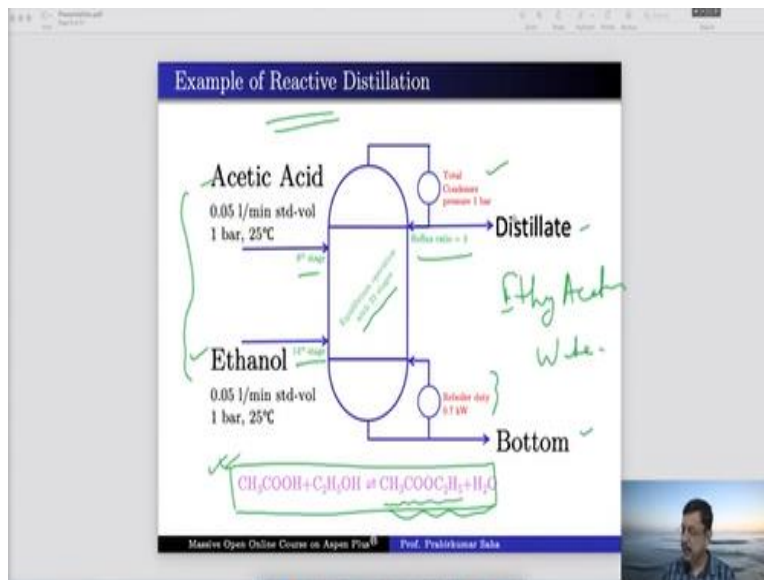


In the multi-stage vapor liquid calculations, it can do for reboiled absorption and reboiled stripping as well in addition to ordinary distillation, absorption, stripping. It is suitable for two phase system three-phase system only in equilibrium mode suitable for narrow and wide boiling system. It can model columns in which two liquid phases and chemical reactions occur

simultaneously using different reaction kinetics for two liquid phases and you know the chemical reactions can occur in distillation that is called reactive distillation.

It can model both random and structured packing a few glimpses have already been demonstrated. And it can also calculate the size and rate columns consisting of trays and or packing's. Now it is not possible for me to demonstrate each and everything but I will cover two things one is absorption column and another is the reactive distillation. These two things will be covered in the next few slides.

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First, we will take the example of reactive distillation. Now this is a column in which acetic acid and ethanol are fed in a column of 23 stages. The acetic acid is sent at eight stage ethanol is sent at 14 stage. Their flow rate and temperature pressure conditions are given the condenser operates at one bar pressure and reboiler duty is given 0.7 kilowatt the reflux ratio is 3. And as it is reactive distillation obviously these two components, they react with each other and form ethyl acetate and water.

So, these two things are product. So, the reaction through which these two are produced is this one. Now we will model this through rad frac.

(Video Starts: 27:44)

For that let us open a new simulation so we have first component acetic acid we can write in this fraction. This is acetic acid, water, ethanol and then ethyl acetate find ethyl acetate so this one you choose add selected compound let us rename it as Eth Ac. Press next we will use UNIFAC method because that is the best property method for this kind of system run it. Go to the simulation block bring in the RadFrac column connect the material first feed distillate product rename it as feed dist bottom. Now here we have two streams.

So, instead of feed we should write acetic acid and we have to look for a second feed through which ethanol will be passed. Now go to next acetic acid input for both acetic acid and ethanol the flow rate and temperature pressure conditions are same. Flow rate is 0.05 liters/minute standard volume and temperature 25 degree centigrade one bar pressure. So, we have to add in these values so 25 degree centigrade one bar standard volume flow rate of 0.05 liters/minute.

Next is ethanol same information 25, 1 standard volume flow 0.05 liters/minute. Press next it will ask for the specification of RadFrac again it is equilibrium model. Number of stages is given 23 stages condenser total condenser and here two information are given one is reboiler duty another is reflux ratio. So, reboiler duty 0.7 reflux ratio 3. So, we will use reboiler duty as 0.7 kilowatt and reflux ratio is 3.

Total condenser somehow it has been deleted then go to streams acetic acid is given at the eighth stage ethanol is given in 14 stage. So, it is 8 and 14 on stage on stage. Then we have pressure condenser pressure is everything one bar. So, now the equations are all balanced it is ready to run. Now if we run it let us see what happens so run is complete, we can see the result. So, this is the stream result we have.

Here you can see that there is no trace of water in the distillate and there is no trace of ethyl acetate in distillate and bottom either. None of these water and ethyl acetate they are in the distillate and bottom. Why so? Because we have never indicated that there is a reaction that is happening. In the inlet we have given only the acetic acid and ethanol we have not entered water and ethyl acetate.

So, there is no water and ethyl acid in distillate and bottom product because we have not stated that there is a reaction going on. We have to state that there is a reaction going on, then only Aspen plus will understand that it is a reactive distillation. So, for that we have to make certain changes. So, let us go back to setup and here we have to add a reaction. So, that reaction begins at stage number 8th where acetic acid is being fed and it ends at 14 because acetic acid is being fed through the 8th stage whereas ethanol is being fed through 14th stage.

So, all the reactions are expected to happen between 8th stage and 14th stage there is no reaction id as such so we have to create a new reaction id let us say r1. Then you will find over here the reaction you have to add a new reaction over here. So, it can be kinetic equilibrium and conversion. For the time being let us take an equilibrium reaction. So, it reacts component acetic acid with ethanol they produce ethyl acetate.

And water here the coefficient is minus 1 and minus 1 because they are reactants and here the coefficient is 1 and 1 because they are product. Press next now the reaction is defined let us run. Now the result is complete you see how much of water has been produced this together it is 0.03488 moles kilo moles in the bottom and 0.0058 kilo moles/hour in the distillate. Similarly, you can combine this is the amount of ethyl acetate that is being produced.

If you want to see the mass flow rate nearly 3.5 kg/hour of ethyl acetate and 0.7 kg/hour of water has been produced through this reactive distillation.

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The image shows a screenshot of a presentation slide titled "Rate based calculations". The slide contains four bullet points:

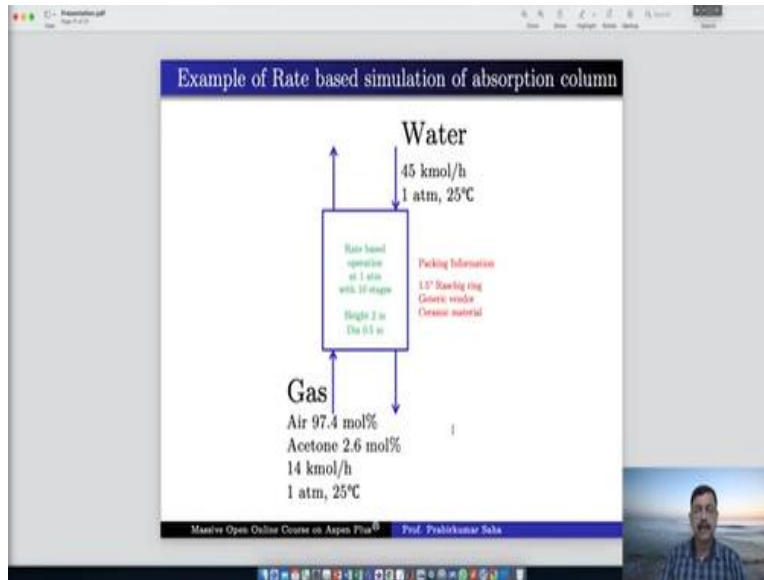
- In rate based simulation, the column can be designed and analyzed completely without the recourse to theoretical stages, tray efficiencies and heights of transfer units.
- It can be designed using only the equipment parameters that can be measured with a ruler.
- Mass transfer rate models use mass (and heat) transfer coefficients, gas liquid contact areas and concentration difference driving force.
- Good correlations for film coefficients and measured equipment geometries (weir heights, passes, open area on trays, random packing size and brand, or crimp angle and crimp height of a structured packing) allow the performance of a real tray or a given depth of real packing to be predicted.

At the bottom of the slide, it says "Master Open Online Course on Aspen Plus" and "Prof. Prabhakar Jaha". A small video inset of the professor is visible in the bottom right corner of the slide.

Till now we were doing only equilibrium-based calculation. Now we will see how the rate-based calculations are done. In rate based simulation the column can be designed and analyzed completely without the recourse to any theoretical stages tray efficiencies and height of transfer units. You can literally take a ruler and measure the height in feet and meters and give that information to Aspen plus and it can calculate on the basis of rate.

Mass transfer rate models are used mass transfer coefficient; gas liquid contact areas concentration difference driving force these are used. And the good correlations for film coefficient and measured equipment geometries like weir heights, passes, open area on trays, random packing size brand, crimp angle, crimp height of the structured packing etcetera. This kind of geometries they allow the performance of a real tray or a given depth of real packing to be predicted.

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To understand that let us take an example of absorption column where rate-based simulation can be done. Let us take this unit here we have a packed column where gas containing 97.4 mole % of air and 2.6 mole % of acetone. Flow rate and temperature pressure condition is given this gas is being passed to this column and it is scrubbed through water pure water whose flow rate and temperature pressure conditions are given as well.

Column is operating on red best at one atmosphere pressure it has 10 stages its height and diameter are given, 2 meter and 0.5 meter. There is some packing information 1.5-inch raschig ring generic vendor ceramic materials all this information is there. Let us try to simulate it.

(Video Starts: 34:39)

For that again we have to open a new simulation. So, we have here air, acetone and water. We will use simple NRTL model. Next run it, go to simulation. Now here in although you are using RadFrac but this kind of icon is not very suitable for you because this icon has condenser and reboiler units with it. Instead, you can use an icon of this nature which does not have any condenser and reboiler.

So, you are using the same model but with a different icon. It is just a cosmetic difference nothing else. All the prevailing equations with the RadFrac they remain the same. So, we have to add in the material. So, there are two inputs one is for gas in and another is for water. There are

two outputs one is for vapour or gas out and this is the liquid out. So, we name them accordingly we will write it as gas in and gas out and this is water and this is liquid.

So, we will place this equation over here. So, this water we will bring it over here and gas in will pass from here. There is no hard and fast rule that you have to do in this manner but these cosmetic changes will make the simulation look better. Now press next so it is asking for inputs for gas in so we know it is air 97.4 so air and acetone 0.974, 0.026. They are all mole fraction and temperature 25 pressure 1 bar and molar flow rate 14 kilo mole/hour.

Next it will ask for water yes water it is asking. The temperature pressure remains same and water is 45 kilo mole/hour. Press next asking for the specification for the RadFrac. Here we will use rate based. Number of stages 10 stages we have. There is no condenser so we have to say none and there is no reboiler so we have to say none. So, as there is no condenser no reboiler so, operating specifications are not required at all.

So, go to streams gas in obviously had it has to be sent from the bottom so it is 10 stage. On 10 stage and water has to be given from top so above and this is on. Go to pressure so here it is not condenser but stage one pressure which is again one atmosphere. Now go to next it is asking for column internals because the rate-based calculation always asks for the column internals, you have to give the length and breadth of all of them.

So, it is again 1 to 10 stages add a new section starting section is 1 and end stage is 10. It is rating internal type packed packing is Raschig ring 1.5-inch Raschig ring generic vendor ceramic material. So, we say Raschig ring generic vendor material is ceramic and dimension 1.5 inch and then packing it is said 2-meter height and diameter 0.5 meter. So, section packed height is 2 meter and diameter is 0.5 meter.

So, the information is complete we can run the simulation now we have to give the rate based modelling. Now here we are yet to give rate-based setup, go to the section all those internals we have to say rate-based calculation, yes. Now it is complete we can run the simulation yes, so we ran it. Now go to the results section so these are the stream results you can see molar flows

acetone out of 0.364 kilo mole/hour 0.287 has gone into the liquid it has been absorbed in liquid only 0.076 kilo mole that is going in the gas out if you see the mole fraction.

So, this is the amount going in the liquid and the liquid 99% is water and in the gas out 96.3 sorry it should be 99% only because 0.001 is only in the liquid. So, 0.963 kilo mole/hour so gas out consists of mainly air and liquid consists of only water almost everything has gone into you can see the mass flow it will look better. Out of 394, 393 kg/hour has done into the gas out for air acetone was only 21 kg/hour out of that 16.69 kg has gone into the liquid only 4.45 kg is going into the gas out.

Now our job is not complete we have to see the hydraulic plot and understand whether there is any flooding and all well. All the trays are in bad shape the entire column is in red and the operating point you can see the operating point is here and this is the bottom line. What is this? This is the minimum pressure drop/unit packed height. That means none of the section of the column it is having this minimum pressure drop/unit packed height.

So, to increase the minimum pressure drop/unit packed height we can change something in the geometry. So, go back to the column section instead of 0.5 meter let us take 0.49 meter and see whether the simulation changes? No, it does not. Go back again instead of 0.49 let us say 0.45 slightly slight changes are observed. Let us try more 0.4 yes, so stage 1 is it has come within the limit stage 2, 3, 4, 5, 6, 7, 8, 9, 10 entire column is now within.

So, this is the crux you can change it further if you want you can use 0.35 and let us see where it goes perhaps it will go in the middle, it is much better for the entire column.

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So, that is how you can play around with the column internals to see how far we can avoid flooding and all those mechanical problems can be solved. Finally, we come to the extract model.

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Extract model

- Number of stages should be mentioned
- Thermal options are either adiabatic operation or stagewise profiles for temperature or heat duty
- Key components have to be mentioned in *extract* phase and *raffinate* phase, referred to as 1st and 2nd liquid phase
- Pressure profile needs to be mentioned stagewise.

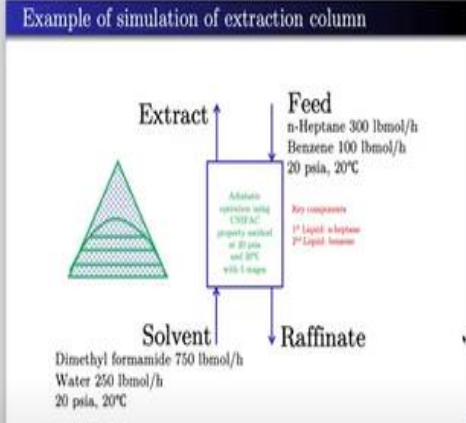
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The Extract model is used for counter current extraction. Here we have to mention the number of stages. We have to give the thermal options either adiabatic operation or stage wise profiles for temperature and heat duty and the key components have to be mentioned in the extract phase or in the raffinate phase referred to as first and second phase liquid and the pressure profile needs to be mentioned stage wise.

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Example of simulation of extraction column



Extract ↑

Feed ↓
n-Heptane 300 lbmol/h
Benzene 100 lbmol/h
20 psia, 20°C


Key components
1st Liquid: n-heptane
2nd Liquid: benzene

Solvent ↑
Dimethyl formamide 750 lbmol/h
Water 250 lbmol/h
20 psia, 20°C

Raffinate ↓

Adiabatic operation using property method of 20 psia and 20°C with 3 stages

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So, to understand it let us take the example for simulation of an extraction column. In the extraction column we have a column having feed of a mixture of n-Heptane and benzene whose flow rates are 300-pound moles/hour and benzene 100-pound moles/hour. Pressure and temperature are given the solvent is a mixture of dimethyl formamide and water. Their flow rate

and temperature is also given the column is operating adiabatically using UNIFAC property method with five stage. The key components are the first liquid is n-Heptane for second liquid is benzene.

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So, to do that we again we open a new simulation. So, we have heptane, benzene, water and dimethyl formamide, yes this is the one. So, let us rename it as diform. Press next we have to use the UNIFAC method press run, go to simulation take the extract block over here material in material out. So here you have to write feed at the top, this solvent this is extract and this is raffinate.

Press next feed material temperature 20-degree centigrade pressure 20 psi all the units are in English units so let us use En. So, pound moles/hour feed heptane 300 and benzene 100, 300 and 100. Next it is 20 degrees centigrade 20 psi solvent dimethyl formamide 750 and water 250, 750 and 250. Now we will use unific method. Press next now we have done the property analysis but we have to check whether the separation through extraction is possible in the first place.

For that we have to get the ternary diagram. So, this is the ternary diagram let us take water as the component 1 dimethyl formamide as the component 2 and benzene as component 3 run the analysis yes. So, we have ternary diagram for water dimethyl formamide and benzene and by watching this ternary diagram we can be sure that the extraction can take place. So, number of stages is five and thermal option is adiabatic.

We can specify temperature profile and heat duty profile as well but we are not going through that complication. Let us choose adiabatic thermal option, key component. For first liquid it is n-Heptane second liquid is benzene so first liquid this is heptane and second liquid benzene. Press next the pressure in the first stage it is 20 psi. Let us now run the simulation. You have to estimate the temperature also stage 1 and 20 degree centigrade now you can run yes. The results are down available.

So, you can see the stream results. So, out of 300-pound moles/hour of heptane 239 has done into raffinate only 60 has done to extract whereas in benzene in case of benzene out of 100-pound

moles/hour 99 has done to extract. So, benzene has almost completely been extracted over there in extract phase. Obviously difrom is the one which has extracted over here the entire mixture has taken benzene out of it.

So, benzene has been extracted from the component and the raffinate it contains only almost it is free of other things 239.709 of hip 10 has gone into the raffinate phase. So, that is how the extract model can work. So, to summarize in today's lecture we have learnt how to use DSTWU, Distl, RadFrac and Extract. These two are for shortcut distillation this is for extraction and this RadFrac is the one which we have learned very thoroughly.

We have not only checked the result of RadFrac along with this shortcut distillation method but we also have done some calculation for reactive distillation and rate-based absorption column with this RadFrac.

(Video Ends: 51:37)

So, I hope this exercise will be very much helpful for you to carry out your own simulations. Thank you.