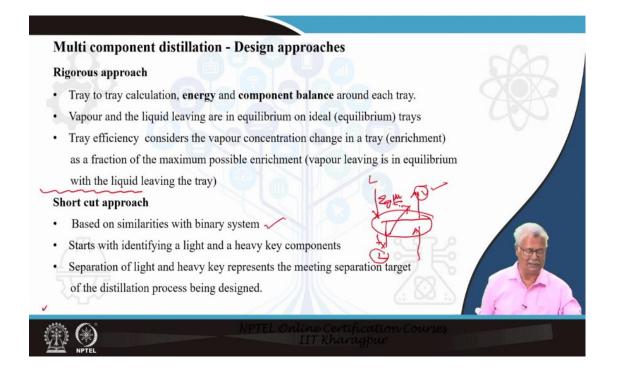
Principles and Practices of Process Equipment and Plant Design Prof. S. Ray Department of Chemical Engineering Indian Institute of Technology, Kharagpur

Module - 02 Lecture - 14 Multi-component fractionation design

Good day to you all. I am going to start today's topic which is Multi-component fractionator design, well you can call it a fractionator or a fractionation system whatever it is. To start with we have to remember that we have covered the binary system distillation design already.

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Now, the first thing that we have in our mind, there are two approaches to multi-component design which is also certainly applicable to binary system designs as well. The first is a rigorous approach. If you are talking about a particular distillation tray here. From the tray, a vapour leaves and a liquid falls off. This liquid and this vapour are in equilibrium. So, that is a fundamental consideration here.

In the case of the rigorous approach what you have, some equations will be telling you that around every tray the enthalpy coming in and the enthalpy going out should match. The

enthalpy comes through the vapour approaching this envelope, and as well as the liquid approach in this envelope and vapour leaving is from the top of this tray itself and the liquid falling off in the tray here.

So, there has to be a balance of enthalpy which is coming in and going out. Exactly in the same way, in the same envelope, there should be a balance of every component that comes in and go out. That means, we first start with an equilibrium approach for an ideal tray. We know that the ideal tray assumes equilibrium which is not possible. So, the concept of tray efficiency has been introduced to you and you already have used and employed it in case of binary distillation.

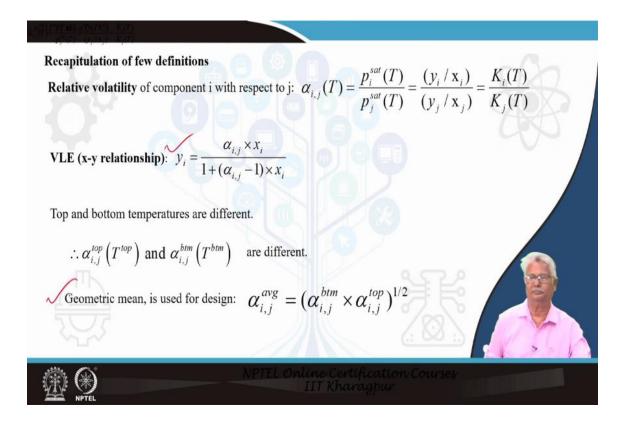
The definition of tray efficiency, particularly the Murphree tray efficiency is simple. It is basically the actual concentration in vapour composition achieved on a tray divided by the maximum it could achieve.

That means, the difference is due to a known approach to the equilibrium on a real tray. Now, this is about the rigorous approach. But we understand that this is going to be rigorous. That means it involves a lot of calculations, a lot of data, and a good amount of mathematical manipulation as well.

So, there are people who thought over it and came up with a shortcut approach. In fact, what we are going to tell you today is a one shortcut method which is typically known as the "Fenske-Underwood-Gilliland" method, but there are other methods as well. Obviously, such systems are based on similarities with the binary system. That means, in a binary system, we know two components are to be separated.

So, the first step in the shortcut approach is to identify two components in the system, the separation between these two attains the goal of the separation of the multi-component system. So, the first step always will start with identifying the light and the heavy component key components, and these are the light and the heavy key. The separation of the light and heavy key represents the meeting separation target of the distillation process being designed.

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We can very quickly recapitulate. We recapitulate the definition of relative volatility in terms of the saturation pressure at a particular temperature, in terms of the molar mole fractions y and x, and also in terms of the distribution coefficient K_i and K_j . So, $\alpha_{i,j}$ expression is what you see here displayed.

The VLE x-y relationship is also given by

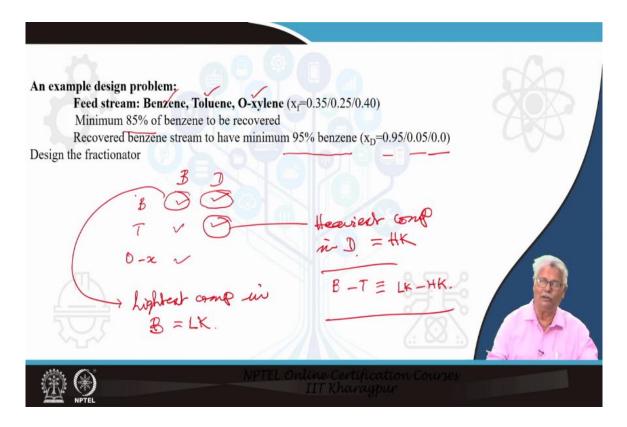
$$y_i = \frac{\alpha_{i,j} \times x_i}{1 + (\alpha_{i,j} - 1) \times x_i}$$

So, if I know alpha, x value, the corresponding y values can be found out.

This is regarding binary, mind it. Then, we also appreciate that the top and the column bottom temperatures are different. Because the top temperature contains lighter components, the bottom temperature has got a higher proportion of heavier components. So naturally the top temperature is less than the bottom.

This makes a difference between the alpha value at the top and alpha value at the bottom. For design the convention is used to use a geometric mean of the alpha at the top and alpha at the bottom as shown here.

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In order to appreciate multi-component design, we start with the design problem. The feed stream contains 3 components. The first is benzene, the second is toluene, and o-xylene; in order of decreasing volatility. I have written here, the feed contains 0.35 mole fraction of benzene, 0.25 mole fraction of toluene, and 0.4 mole fraction of o-xylene.

The target of separation tells us that minimum of 85 % of the benzene has to be recovered. The recovered benzene has to have a minimum of 95 % benzene purity. So, what we could decide is mole fraction of the distillates are going to be 0.95 for benzene. I decide that I am not going to send any o-xylene up. So, naturally, the rest amount is toluene. There is no o-xylene. So its mole fraction is here is 0.

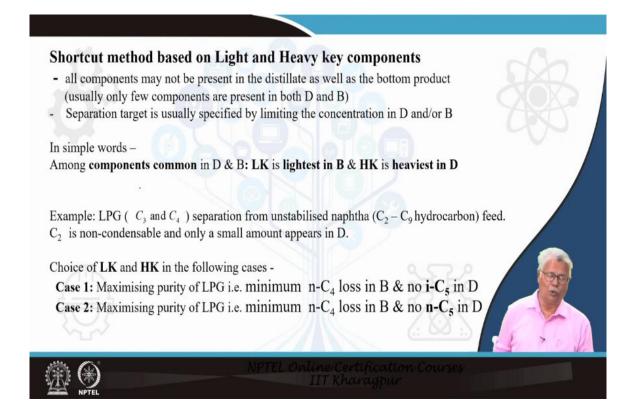
The problem is designing the fractionator. So, what we find is we have benzene, we have toluene, we have o-xylene. If I look here the B and the D here benzene is available at the distillate, toluene is available at the distillate. We recovered only 85 % of the benzene. So,

the rest amount of benzene will be at present in your bottoms. Naturally, benzene is present in the bottoms the heavier ones will be available there too.

So, what we find here is that the lightest component in the bottom. What is it called? It is called the light key. What is this? This is the heaviest component in D. What is that? This is called the heavy key and that is the convection. So, if you can achieve a separation between benzene and toluene which are basically the light key and heavy key, the separation target will be fulfilled. That means, we will be sending we will have common components between the bottoms under distillate, but our target will be fulfilled in this way.

Let us look at fixing these light and heavy components in slightly more detail.

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To start in a formal way we understand and appreciate that all components may not be present in the distillate as well as the bottom product, that we have seen already. Usually, only a few are common. The separation target is specified by limiting the concentration in D or B or both at times. In simple words, among the components common in D, the light

key is the lightest in B and the heavy key is the heaviest in the distillate. We go for an example, another example.

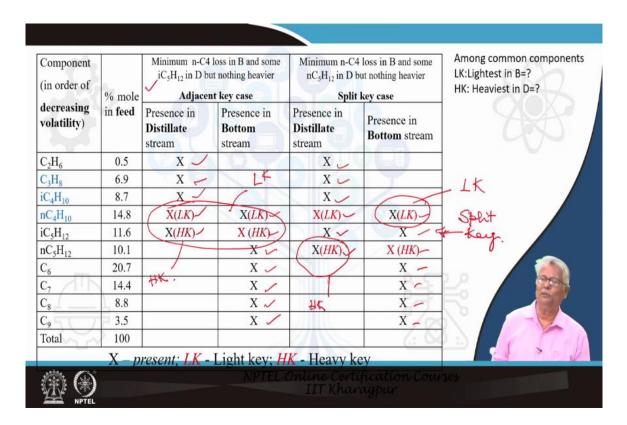
We talk about a column in which the target is to separate LPG, mostly C3 and C4 hydrocarbons from a mixture of naphtha which contains C2 to C9 hydrocarbons. That means it is an unstabilised naphtha feed.

During separation, one thing is sure if I am going to use it, use this separation to be carried out in a fractionator. C2 is the lightest. Possibly that is not going to condense there, because if I have to condensate to I either require a very high-pressure column or I need a cryogenic column.

So, quite likely it will be so, that I will be losing the ethane as vapour from my reflux drum. You know what the reflux drum is already, and possibly along with it, I will be losing a certain amount of C3 as well which is propane.

Now, we have two cases here.

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We move to the next slide here, in fact, have a look at a table here and see the composition of the feed being listed here starts with ethane and end with C9. It is in the order of decreasing volatility and the composition is also known.

The first thing you will see we are talking about this particular case, which means case 1, which I have referred to in my last slide. Here what we have is we decide that my top product is not going to contain any nC5. So, basically, my top product is going to contain C_2H_6 , C_3H_8 , iC_4H_{10} , nCH4, iC_5H_{12} . The bottom product will definitely contain the rest. It will start from this one and continue up to C9 component.

So, in this particular case, we note here very clearly that the common components are nC_4H_{10} and iC_5H_{12} . So, what will be the light key in this case? The light key is what? The light key is the lightest in the bottom product. So, n-butane is going to be my light key. The heavy key is the heaviest component in my distillate, so iso-pentane is going to be my heavy key.

Now, the same separation, that means, with the same feed, the top product being LPG again which is expected to be primarily C₃ and C₄. I consider it in a different case. What do I have here? I have here I am going to accommodate a certain amount of nC5 in this also. So, can I say or can you appreciate at this particular point that the LPG which is a distillate stream here, in the left case of the case 1 is not going to contain any n C 5, in the right case, case 2, it is going to contain nC5.

So, your LPG is going to be purer in the first case and is to be relatively impure in the second case. Quite naturally, you have an extra yield of LPG volume of production in the second case. Now, obviously, again my distillate will be containing these, these, these, and up to my nC_5H_{12} . What we have is, we also have these components at the bottom. Now, instead of just two common components between the D and the B, we have 3 here.

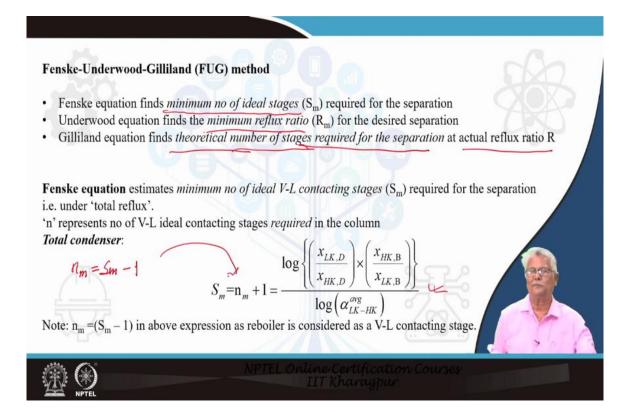
Now, we go and identify the light and the heavy key, the light key is supposed to be this. So, this is going to be my light key. Why it is a light key? Because it is the lightest component in my bottoms. This is going to be my heavy key because this is in this, this in this case is going to be the heaviest component in my distillate.

Now, apart from the light and heavy key, you have at least one component which is in between, which is present in both. So, this is called a split key which has volatility between

the light and the heavy. So, naturally, all key components will be present in both distillate as well as the bottoms. The light key and the heavy key will be the extreme ones. The split key will be present in both as well.

Normally, the split key is considered to be distributed between the distillate and the bottoms according to their volatility. We will see later on when we come to the calculations.

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The technique which I have mentioned at the beginning is the Fenske Underwood Gilliland method. We talked a lot about the minimum number of ideal stages required for separation; we did so. So that we designate it by S_m . We also have talked about the minimum reflux ratio for the targeted separation designated by R_m . Sometimes we say R_m , sometimes we say $R_{minimum}$.

The Gilliland equation is the most important equation at the end. This is going to give us that the actual number of theoretical stages, ideal stages, required for the separation at a particular reflux ratio of R, which is more than R_m . Because R_m is a minimum required reflux, your actual operating reflux R has to be higher than R_m .

There is one more thing that is also there that we will see later on that is how to split the total number of stages which is S, which is found out from the Gilliland equation into the stages above the feed tray and the stages below the feed tray. At the same time, this is going to tell us the location of the feed tray as well.

Now, we look at the Fenske equation. We have the case of a total condenser given here. Here it says S_m , which is the number of minimum theoretical stages required for the separation is equal to a log of something divided by log of alpha. Quite naturally, the number of stages required would depend on the relative volatility, it will also depend on the concentration required and the top and the bottom products of the light and the heavy key. So, this is expectedly and known expression or something like this.

Now, if you look at the distillation system we will find there is one vapour-liquid contact that is happening in your reboiler. So, if you have S_m number of stages, the number of stages of contact that you have to provide inside your column or tower is less than S_m by 1. That means, basically n_m is equal to (S_m-1) , which is again reflected here in the same equation as an additional term.

This was the case of the total condenser.

Fenske equation

Partial condenser

Since a partial condenser provides one stage of V-L contacting, the no of ideal stages to be provided in the column in this case diminishes further by 1.

Finally, one additional stage considered in the column as V-L contacting is expected to be poor on the feed tray and corresponding vapour enrichment is neglected.

Underwood equation estimates the minimum reflux required for the separation. When feed is at the bubble point (q=1)

$$R_{m} = \frac{1}{\left(\alpha_{LK-HK}^{avg} - 1\right)} \left[\frac{x_{LK,D}}{x_{LK,F}} - \frac{\alpha_{LK-HK}^{avg} \times (1 - x_{LK,D})}{(1 - x_{LK,F})} \right]$$



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We can have a partial condenser also. In a partial condenser, it provides one more vapour liquid contracting stage. So, what happens is the number of trays to be provided inside the column or tower has to be further reduced by 1, is diminished further by 1.

Now, in a distillation column typically you may or may not think that the, I mean rather what happens is the contacting on the feed tray is not usually very proper. You have a distribution problem, you have condensation of some vapour component coming in contact with feed and such things. So, what happens is; if you do not take credit for this you have to increase the number of stages which is required in your column by one more.

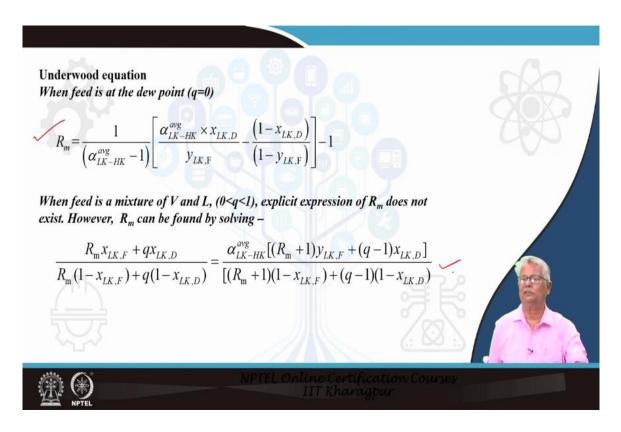
So, definitely, in that case, you will be adding one more to the n_m value that you have finally arrived so far. So, one thing is true up to this particular point, we have decided on n_m or the minimum number of ideal stages or ideal trays that I have to produce and that I have to provide inside my tower or the column itself.

What is the next thing to be done? We need to find out the R_m , which is the minimum reflux required for the separation. Now, you definitely remember the binary system; how did we locate the point of minimum reflux for a particular separation?

There we required the composition of the feed as well because it was a point where on the equilibrium line, the equilibrium where the two operating lines stripping section operating line and the rectification of section operating line they came and met.

So, quite naturally the expression of R_m which is given by the Underwood equation would contain parameters related to the feed and parameters related to the distillate as well. Certainly, the equilibrium will be represented by the alpha term. So, we can appreciate very well why these terms appear in the expression of the R_m . At this particular stage, all these parameters are known and you can estimate an R_m in the problem.

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This is a case where the R_m is found when the feed is at its dew point. We also know that the feed line and the two operating lines in the case of the binary are made on the equilibrium line. That depended on the value of q or the slope of the feed line or q line or f line whatever you may call. So, quite naturally your R_m should also be a function of q.

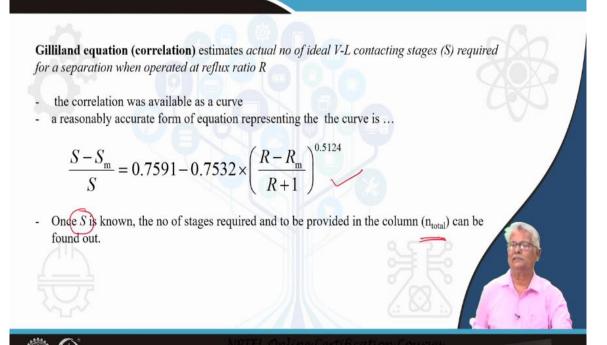
So, in this specific case q is equal to 0, and quite naturally you need not have a value of q here. In the previous case, the q value was 1 which was put here, and you had an expression direct explicit expression for R_m . In the previous case, where the feed was at its bubble

point, and in this case, what you have is the explicit expression of $R_{\rm m}$ with the feed at its dew point which is vapour feed.

When it is a mixture, the expression is rather complicated and you cannot have an explicit expression in R_m , but however, there is a relationship that can be solved by trial and error. If I know my q, if I know my x values, if I know my alpha by trial we can solve this and find out my R_m .

So far what we have found out is, we have found out a number of theoretical stages that we have to provide in my tower, within my tower itself. We also have found out for this particular separation extent; what is required minimum reflux under a particular feed condition with q having a value of 0 or 1 or some other value of q.

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We again have something very similar to what we have done earlier. We had assumed a particular value of R/R_m . We had a procedure based on the construction of those triangular steps, and we found out the number of theoretical stages required for the separation. In fact, Gilliland gave us a correlation in the graphical form originally whose mathematical form is here. This is the mathematical form.

This has been found out empirically, and it relates the minimum number of theoretical stages S_m to the real number of stages corresponding to R. That means, S corresponds to R reflux ratio, and S_m corresponds to R_m the other minimum reflux ratio. This is the expression.

$$\frac{S - S_m}{S} = 0.7591 - 0.7532 \times \left(\frac{R - R_m}{R + 1}\right)^{0.5124}$$

Since we already have found out S_m, and R_m, so definitely is possible for us to know the value of S. Up to this is fine; that means, we know the total number of theoretical stages required. From this we will be subtracting and adding 1, for different reasons, for the reboiler, condenser, partial condenser, taking credit for feed tray. We definitely will be knowing the number of trays required in total for the desired separation within the column itself.

Now, quite naturally if I have to ask for the column design finally, I have to specify the location of the feed. That means, the number of trays that appear in the stripping section and the number of trays that appear in the rectification section.

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Feed tray location

- Approach based on Fenske equation
 - considers the rectification and the stripping section as independent columns
 - compares the ratio of no of theoretical stages at total reflux for the rectification (S,) and the stripping (S.) section

$$\frac{S_r}{S_s} = \frac{\log[(x_{LK,D}/x_{HK,D}) \times (z_{HK,F}/z_{LK,F})]}{\log[(z_{LK,F}/z_{HK,F}) \times (x_{HK,B}/x_{LK,B})]}$$

Based on the above ratio, n_{total} can be apportioned to n_r and n_s . Then, applying and overall efficiency: $n_r^{actual} = n_r / \eta_o$ and $n_s^{actual} = n_s / \eta_o$. n_r^{actual} and n_s^{actual} are rounded off to the next higher integer for a conservative design output.



This can be done in two ways. The first thing is an approach based on the Fenske equation. The Fenske equation considers the rectification and the stripping section as the independent columns. That means, what you had is a feed, from the top you had a distillate (D), from the bottoms you have residue (B).

So, what you consider here is column 1, this is column 2. That means, for column 1 the top product is x_D , the bottom product composition in column 1 is $x_f(Z_f)$. In the case of column 2, the top product is $x_f(Z_f)$ and the bottom product is x_B .

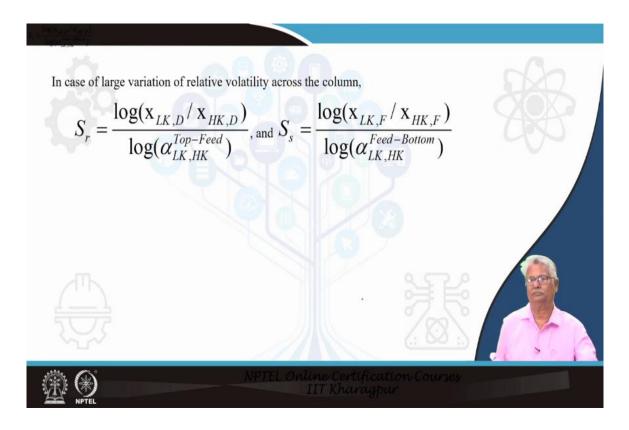
Now, based on this consideration if we look at the number of theoretical stages required; the minimum number of theoretical stages required, the ratio of those two in the rectification section which is column 1 and the stripping section which is column 2 we have an expression like this. Here you will note that we are using the values of the composition of the feed quite naturally.

This is valid at a composition of minimum number of tray because this is based on the Fenske equation. For Fenske equation is valid for the total reflux or the minimum number of theoretical stage conditions $S_{\rm m}$.

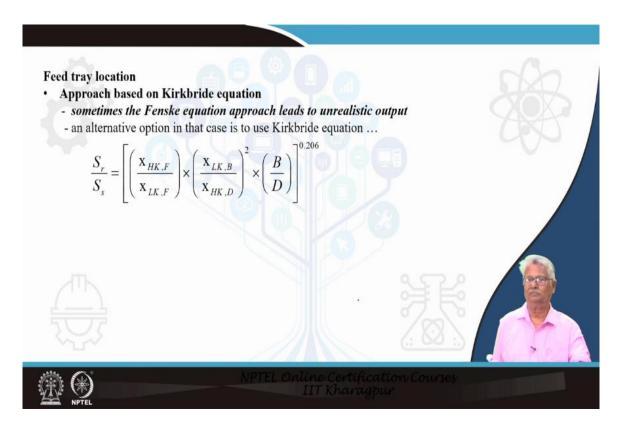
We assume that the ratio is the same. So, what we do next is based on this above ratio we split in total, and after we have done that we find out the number of rectification stages in stages to be provided inside the column divided by the overall efficiency and find it out by after rounding off.

The same thing we do for the number of theoretical stages to be offered for the actual separation when the actual separation has got an overall efficiency of η_0 to be this. The actual number of stages is found out by rounding off to the next higher value.

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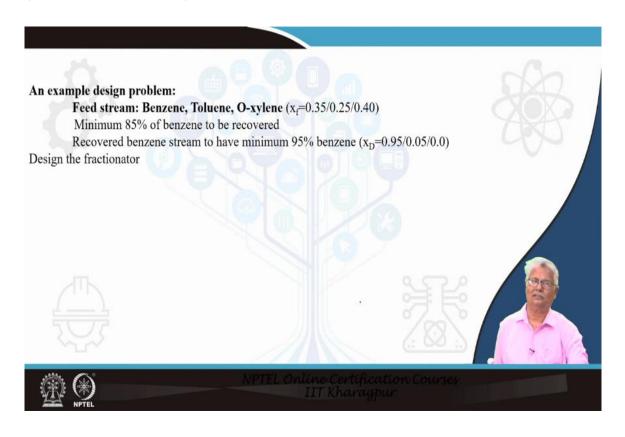


In case we have a large variation of relative volatility across the column, we do not have the previous expression, we have a modified expression that looks like this. (Refer Slide Time: 26:34)



Sometimes, the approach based on the Fenske equation does not give us the desired realistic result. In such a case, an alternative equation proposed by Kirkbride is used which is again defined the same way. It involves a compilation of the bottoms, the composition on the top the feed composition, in terms of the light and the heavy key, and also the yield of the bottom and the distillate streams.

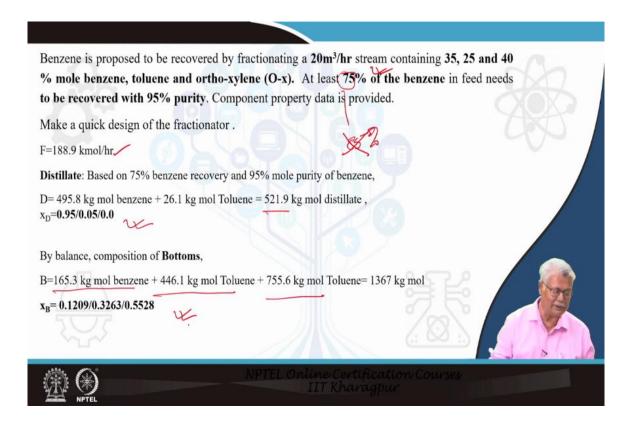
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So, we have an overview of the multi-component distillation and it's time that we have a look at the example design problem once more. The feed string; I just repeat the problem here the feed stream, benzene, toluene, and o-xylene has got composition mole fractions of 0.35, 0.25, and 0.4.

Minimum 85 % of the benzene to be recovered, with a minimum purity of 95 % and we have decided that my distillate composition is going to component no amount of o-xylene. So, the composition is 0.95, 0.05 and 0; and the fractionator has to be decided.

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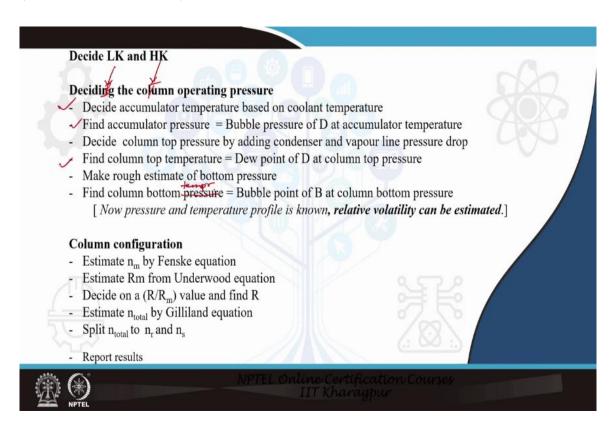


This is the full statement. It is in fact, a realistic problem with a feed rate of 20 m³/h and the same thing is given here. Only thing the 75 is wrongly written here, it should have been 85 %. We are going for a quick design now. We know the feed composition. We know the molecular weights. So, my feed is 188.9 kmol/h.

We simply have found out, the composition of the distillate and we have found the ones here. I will just make one more correction here that this is not 85, this is worked out based on 75 %; 85 % is that problem which was given in the first instant, right at the beginning of this particular lecture.

Now, we know the distillate composition which is here, the quantity of is also known and this is 0.95, 0.05, and 0. By balance the composition at the bottom is also known which is this much of benzene, this much of toluene. The corresponding x_B values are also given here.

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Basically, to conclude let us have a look at the steps require to complete the problem here. The first thing is finding out the light key and the heavy key that we have already said. My light key in this particular case is going to be my benzene and my heavy key in this case is toluene because and it is a case of adjacent key, because they appear in the same sequence one after another in the order of volatility.

The first step after this should be deciding the accumulated temperature based on the coolant temperature which is used in the condenser. Because the condenser outlet is going to have the temperature which is there in your accumulator. There usually has to be a temperature gradient of anything between 10 to 20°C, for the driving force to remain in your condenser.

So, if you are using a coolant cooling water that is available at 33°C and returned at around 45°C, your expected accumulator temperature is going to be something around 43, 44, 45°C or it could be slightly higher even.

The next is finding the accumulated pressure which is simple. Rather, we all know that the distillate is at its bubble pressure at the accumulated temperature within the accumulator

itself. We know that the distillate composition, so we find out the accumulated pressure by as by evaluating the bubble pressure of the distillate.

Next what we do is, we are required to find out the column top pressure. The column top has to be at a slightly higher pressure, because the vapour has to flow from the column top through the overhead lines for vapour, go to the condenser and finally, come out of the condenser as in the condensed form. Typically, the pressure drop will be of the order of around 0.3, 0.4 kg/cm² which is added to the accumulated pressure to have an estimate of the column top pressure.

The column top temperature is nothing but the dew point of the distillate at the column top pressure. We know the column top pressure we just found it out. So, what we do is we find the dew point of the composition D at this pressure and we note this as the column top temperature.

We need to have initially and a rough estimate of the column bottom pressure itself now. Suppose we decide that we are going to you; we expect around 18 to 20 trays in this type of separation. We consider roughly about 50 mm of water column per tray drop. At this drop to the column top pressure, and we have an estimate of the column bottom pressure itself.

Now, the column bottom temperature is the bubble point temperature of B at a column bottom pressure. So, what we know now is the entire column profile of temperature and pressure. We know the relative volatility at the top and the bottom condition. We can use a design relative volatility estimate as a geometric mean of the column top and the column bottom relative volatilities, between the light key and the heavy key.

Obviously, once we have configured our column the steps are simple using the formula which has already been told to you, we evaluate n_m as per the Fenske equation, after definitely correcting for the plus 1 and minus that we have talked about earlier. We estimate the R_m from the Underwood equation which is the minimum reflex required for the separation.

We decide on an R/R_m value above 1, maybe 1.1 or so. Find out the R corresponding to that particular R/R_m of 1.1 maybe as a first trial. We find out the n_{total} required that is the total number of trays required as for the Gilliland equation and the efficiency assuming

around 0.7. We split this n total to the number in the rectification section and the stripping section and we report the results.

So, this is going to be the way we approach is distillation column problem which has got multiple components. We have considered only 3 components here, but there could be several. But the approach is similar because it is based on the similarity with the binary. Just only the light key and the heavy key are identified and are worked upon.

I think with this, I will conclude the topic on the multi-component fractionators. The next topic to be taken up will be Batch Distillation.

Thank you.