**Plant Design and Economics**
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Lecture No -38
Design of Multi–component Distillation Column: Short Cut Method

Welcome to lecture 38 of plant design and economics. In this lecture, we will talk about the design of a multi component distillation column by short cut method.

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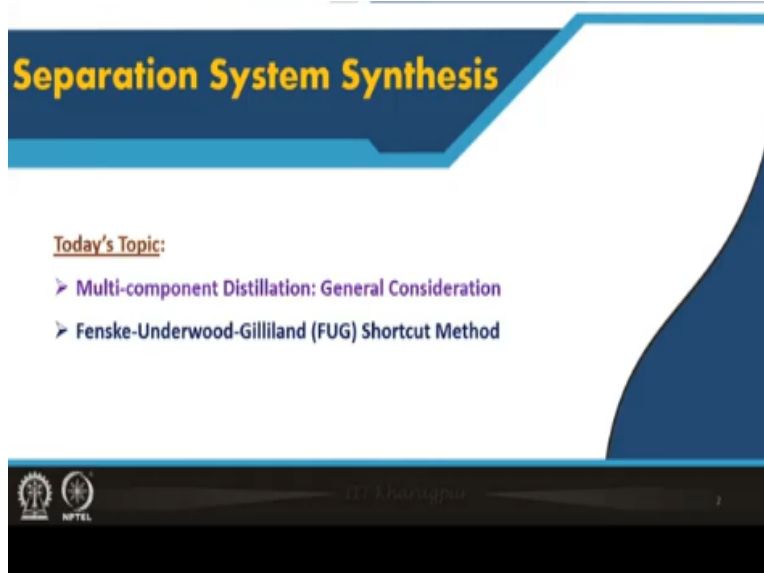
So we will first talk about some general considerations about Multi-component distillation design and then we will talk about a shortcut method known as Fenske-Underwood and Gilliland short cut method.

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Distillation Column Design: General Steps
1. Specify the degree of separation required: set product specifications.
2. Select the operating conditions: batch or continuous, operating pressure.
3. Select the type of contacting device: plates or packing.
4. Determine the stage and reflux requirements: the number of equilibrium stages.
5. Size the column: diameter, number of real stages.
6. Design the column internals: plates, distributors, packing supports.
7. Mechanical design: vessel and internal fittings.

The principal step is to determine the stage and reflux requirements. This is a relatively simple procedure when the feed is a binary mixture, but can be complex when the feed contains more than two components (multi-component systems).

Now, let us first look at the general steps for design of a distillation column. We need to specify the degree of separation required; that means we have to set product specifications. We have to select the operating conditions, first decide on whether it will be a batch process or continuous process decide on operating pressures etcetera. Select the type of conducting devices, are you going to use plate or tray type distillation column or pack type distillation column?

Determine the stage and reflux requirements; that means determines the number of equilibrium stages or ideal stages, size the column; so determine the diameter of the column, determine the number of actual stages or real stages, design the column internals such as plates, distributors, packing supports, for fragment column etcetera. And then finally do the mechanical design; vessel and internal fittings.

Now the principal step for the design of a distillation column is of course the determination of the number of stages or trays and the reflux requirement. This is a relatively simple process when we are talking about separation of a binary feed mixture, but it can be quite complex when the feed contains more than two components, that means when you have a multi component mixture.
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Binary Distillation Column: McCabe Thiele Method
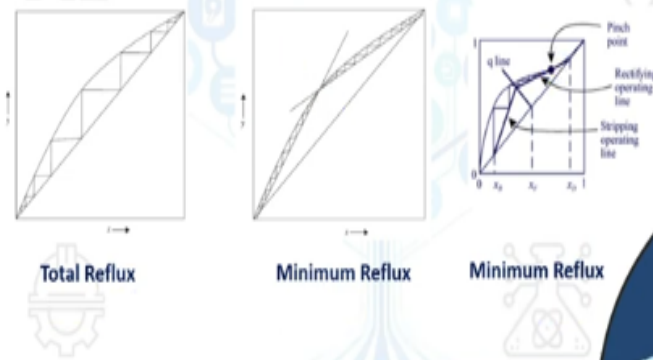
Total Reflux — Minimum Reflux — Minimum Reflux

We are familiar with McCabe Thiele method for determination of number of stages and reflux requirements, for binary mixtures. So you are familiar with total reflux conditions where no product is withdrawn, there is no feed. Minimum reflux; when the number of trays becomes infinite, here the pinch happens because the feed line passes through this, the pinch may also happen due to the shape of the equilibrium curve. So this also gives an infinite number of stages and corresponding minimum reflux can be found out.

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Binary Distillation Column: Optimal Reflux Ratio
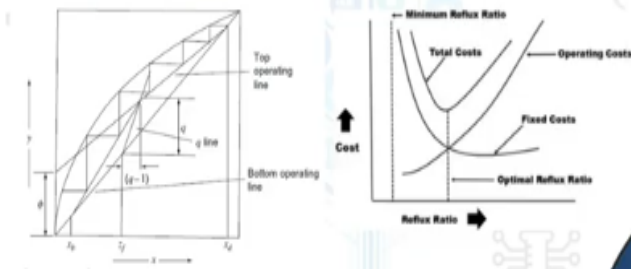
So you are familiar with determination of this number of trays by drawing the steps within the space available between the equilibrium curves and the operating lines for the rectifying sections and the stripping sections. And then finally you are also familiar with the determination of the

optimal reflux ratio which can be obtained from a plot of total cost versus reflux ratio and as you know as the reflux ratio increases the fixed cost decreases due to requirement of fewer number of stages in the column.

But as you increase the reflux ratio the heat load increases, the operating cost increases. So the total cost, which is a combination of these two sources, a minimum software which corresponds to optimum reflux ratio. Now all these things are relatively simpler for a binary distillation column.

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The problem of determining the number of stages and the reflux requirement for multi component distillation columns is not as straightforward, in fact it is much more complex than for binary mixture. Note that, with a multi component mixture, fixing one component's composition does not uniquely determine the other component's composition and the stage temperature. When the feed contains more than two components, it is not possible to specify the complete composition of the top and bottom products independently.

The separation between the top and bottom product is usually specified in case of multi component distillation by setting limits on two key components, between which it is desired to make the separation. So we specify two components, we call them key components and between these two components it is desired to make the separation. So we will see these key components
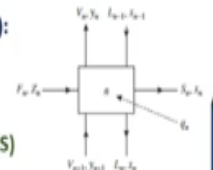
in some more detail now.

There are broadly two design approaches for multi component distillation columns; one is rigorous approach another is short cut approach. Look at these diagrams, let us say this represents the nth tray in the distillation column. So what you see is all the streams that may be around the nth distillation column, liquid stream, vapor steam, may be the feed stream, may be the side stream and also represents the native flow.

In the case of rigorous approach for each stage we solve material balance, equilibrium relationship, such as y i equal to k x i summation such as sum of mole fractions equal to one and heat balance equations. These equations are collectively known as MESH equations, M for material balance, E for equilibrium relationships, S for summation and H for heat or energy balance equation. So for each stage including the reboiler and condenser we can solve these MESH equations, the solutions of these equations form the basis of the rigorous methods.

It is a very detailed calculation where you solve mass balance equations, energy balance equations, equilibrium relationship, as well as summation relationship for each stage, including reboiler and condenser. These calculations are almost always done these days using process simulators such as ASPEN, HYSYS, ChemCAD, gPROMS etcetera. Because manual calculations will be extremely tedious and we have very efficient process simulators and with the

advent of white space computing facilities.

The process simulators are all used these days for designing of distillation columns through rigorous approach. Whereas shortcut approach is relatively simpler, in fact, all such process simulators also have shortcut approaches as different modules. Various shortcut methods are developed to simplify the task of designing multi component distillation columns before the widespread availability of computers and such process simulators.

But shortcut methods are still useful for preliminary design as well as these results of shortcut methods are often used as initial starting point or initialization of computer based solutions.

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Now, let us understand what do you mean by key components? As you pointed out before for the multi component distillation process, we must first select the two key components between which it is desired to make the separation. These two key components are known as light key and heavy key. Light key, the components to be kept out of the bottom product. The light key is the component which must be kept out of the bottom product and the heavy key is the component to be kept out of the top product.

So a light key is the component to be kept out of the bottom product and a heavy key is the component to be kept out of the top product. The keys are known as adjacent keys if they are

adjacent in a listing of the components in order of volatility. So arrange the components according to their volatility and in almost all cases this will correspond to the normal boiling point. Keys are known as adjacent keys if they are adjacent, that means they assume adjacent positions in this listing of the components in order of volatility.

And split keys or non-adjacent keys if some other component lies between them in the volatility order. So split keys or non adjacent keys refer to the case where some other component lies between these two keys. A separation between adjacent keys is also known as a sharp split, a separation between adjacent keys is known as a sharp split, while a separation with nonadjacent keys is known as a sloppy split.

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Key components must be present in both the overhead and bottoms, so that by specifying the recovery of the keys, we can specify the extent of the split. Product specifications are generally expressed in the form of recovery specifications. For example, we specify the 75% of butane in feed exists in the overhead. Calculations of mole fractions require prior knowledge of how all the components are distributed between the products.

So using mole fractions will require the knowledge of how all the components are distributed between the products. The non-key components that appear in both top and bottom products are known as distributed components. While the non-key components that are not present

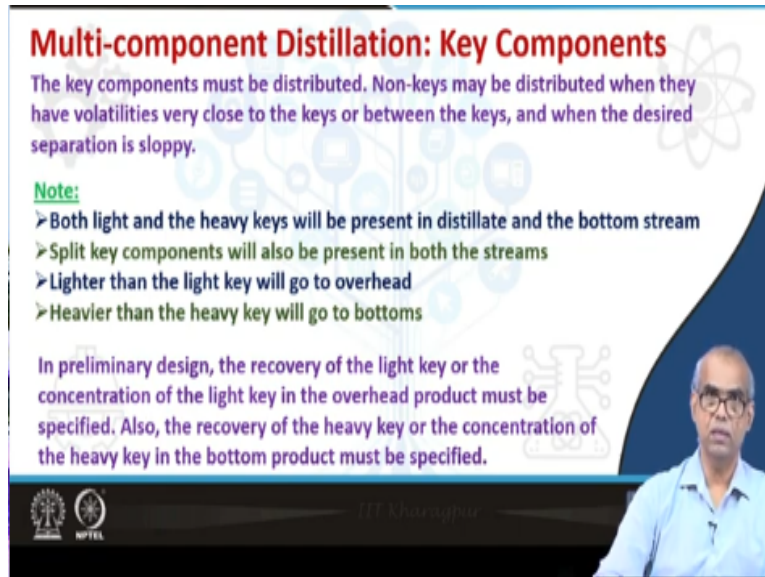significantly in one or other product are known as non-distributed components.

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The key components must be distributed. Non-key is maybe distributed when they have volatilities very close to the keys or between the keys and when the desired separation is sloppy, so for sloppy split. Let us summarize, both light and the heavy keys will be present in distillate and the bottom stream. Split key components will also be present in both the streams. Lighter than the light key will go to overhead. Heavier than the heavy key will go to bottoms.

So lighter than the light key will predominantly go overhead, heavier than heavy key will predominantly go to bottoms. In preliminary design, the recovery of the light key or the concentration of the light key in the overhead product must be specified. Similarly the recovery of the heavy key or the concentration of the heavy key in the bottom product must also be specified.

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Key Components: Example: LPG Production

Component	Mol% in Feed	
C_2H_6 (Ethane)	0.8	
C_3H_8	6.61	
iC_4H_{10}	8.67	
nC_4H_{10} LK	14.77	Volatility Decreases
iC_5H_{12} HK	11.61	
nC_5H_{12}	10.06	
C_6	20.84	
C_7	14.4	
C_8	8.77	
C_9	3.47	

Feed to debutanizer to produce LPG as top product

LPG is primarily a mixture of C_3 and C_4 hydrocarbons. Ethane (C_2H_6, lightest component) does not condense in overhead condenser and is purged out.

To maximum the yield of LPG, split the feed stream as:
Distillate: all of nC_4H_{10} and lighter components
Bottom: all of iC_5H_{12} and heavier components

However, in practice, nC_4H_{10} and iC_5H_{12} will be partially separated and will appear in the top as well as the bottom product.

According to separation target:
Light Key: nC_4H_{10} , Heavy Key: iC_5H_{12}

Let us now look at an example of LPG production to demonstrate the concepts of key components. So what you see in the table is a feed mixture to the debutanizer column which produces LPG as the top product. Note that LPG is primarily a mixture of propane isobutane and butane, basically C3 C4 hydrocarbon mixture. The lightest component ethane does not condense in the overhead condenser and is purged out.

So if I want to maximize the yield of LPG, we should split the feed stream as follows such that in the distillate all of C4 and lighter components go to the display and all of isopentane; that means C5 hydrocarbons and heavier components go to bottom. So this goes to distillate and this goes to the bottom. So to maximize the yield of LPG this plate is desirable because these C3C4 hydrocarbons are essentially LPG mixture.

Of course in practice the n-butane and isopentane will be partially separated and will appear in the top as well as bottom product. According to the separation target my light key will be n-butane and heavy key will be isopentane. So these two components will be my light key and heavy key respectively.

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Now let us discuss about various equations which are related to the design of multi component distillation columns. We will start with the Fenske equation which gives us a minimum number of ideal trays, that means we are talking about our distillation column operating under total reflux condition.

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You are perhaps familiar with the Fenske equation for binary distillation columns. The Fenske equation predicts the number of ideal stages for a specified binary separation of total reflux through this equation. Note that if these number of plates, like 1, 2, 3 etcetera up to n, then it is possible to relate the mole fraction of A, divided by mole fraction of B in the vapor around tray 1 with the mole fraction of A and mole fraction of B in the liquid in the bottom through this

relation.

Where alpha 1, alpha 2 all these alphas represent relative polarity around each trays, R represents reboiler here. Now Assuming a total condenser and constant relative volatility we can rewrite this equation as this, where you are relating the mole fractions or the concentrations of the compositions in the distillate with the compositions in the bottoms through this Fenske equation. So here N minimum is the minimum number of theoretical stages, including the reboiler.

Alpha A B is the relative volatility between A and B. So subscript D represents distillate and subscript B represents bottoms. So this is the Fenske equation as we write for the binary distillation column, now we can extend this relation for multi component mixture as well as. So the Fenske equation can also be used for multi component distillation columns.

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So to use the Fenske equation for a multi component system, we must choose two reference components i and j. Note that for a binary mixture, it was written between components A and B. Now when you have a multi components system we can make use of the Fenske equations, but now it has to be written for any two reference components, say i and j from your multi component system. So this x A by x B in distillate can be written as xi D by x jD or x i by x j in the distillate.

That means composition or concentration of ith component in the distillate divided by

concentration of jth component in the distillate. Similarly, x iB x jB will represent concentrations of ith component in the bottom and concentration of jth component in the bottoms. Alpha ij represents relative volatility between the components and N minimum is the number of ideal stages including the reboiler. So this is a straightforward extension of Fenske equations from binary systems to multi component systems.

This equation we can also write in alternative forms. For example, we can also write the Fenske equation in terms of molar distillate flow and molar bottoms flow, so here d represents molar displace flow and b represents molar bottom flow. We can also write the Fenske equation in terms of recovery of component in distillate or recovery of component in bottoms. So in these equations r represent the recovery of components. For example, r i D represents recovery of component i in distillate, r j B represents recovery of component j in bottoms, so all these forms can be used.

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Now, how do I find the minimum number of ideal trays or equilibrium stages by using the Fenske equation? As we discussed for multi component systems the separation required will be specified in terms of key components, that means light key component and heavy key component. Let component i represent the light key component and j represent the heavy key component. So, the Fenske equation that you have seen in the previous slide in terms of x i, x j can be written in terms of x of light key or x of heavy key.

So we can write this equation where i and j are chosen as light key and heavy key respectively. Then we rearrange and then take logs and then we get this equation, note that you take a log and you will get this equation. So this equation tells us how to compute the minimum number of trays under total reflux conditions. Note that this log of alpha between light key and heavy key can be computed either using these or it may also be computed using this.

So the alternate forms in terms of molar distillate flow, molar bottom flow or the recovery of light key components and the recovery of heavy key components.

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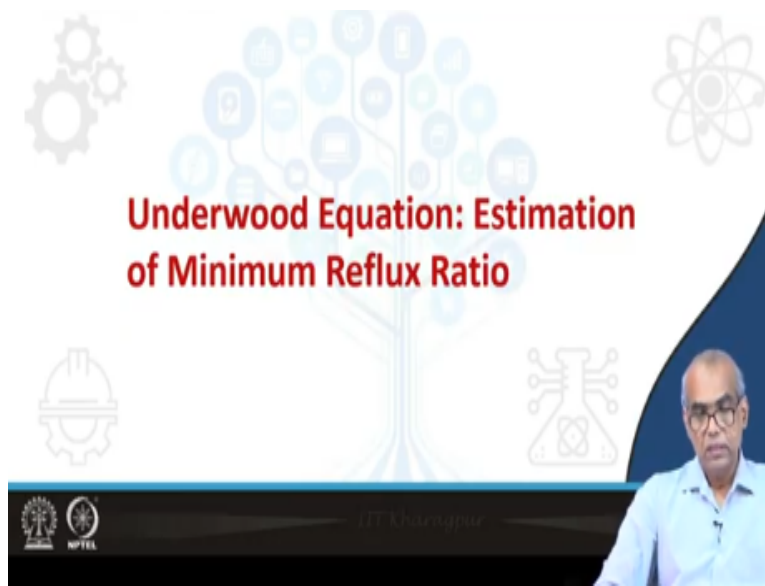
Now we will consider the underwood equation which is useful for estimation of minimum reflux ratio. So in the Fenske equation, we applied under total reflux conditions, that was one extreme. Now let us consider the other extreme conditions where the displacement column will be operated under minimum reflux ratio, under these conditions we will apply an underwood equation. So applying the underwood equation, we can find out the minimum reflux ratio.

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Underwood Equation: Minimum Reflux Ratio

Underwood Equation:

$$\sum \frac{\alpha_i x_{i,D}}{\alpha_i - \theta} = R_{min} + 1$$

α_i = the relative volatility of component i with respect to some reference component, usually the Heavy Key

R_{min} = the minimum reflux ratio

$x_{i,D}$ = concentration of component i in the top product at minimum reflux

Here, θ is the root of the following equation:

$$\sum \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 1 - q$$

Here, $x_{i,f}$ = the concentration of component i in the feed, and

q = (Heat required to vaporize to 1 mol of feed)/(Molar latent heat of feed)

Feed Condition	Value of q		L – V Mixture Feed	$0 < q < 1$
Saturated Liquid Feed	$q = 1$		Subcooled Liquid Feed	$q > 1$
Saturated VapourFeed	$q = 0$		Superheated Vapour Feed	$q < 0$

The under root equation is written as this, alpha i x iD divided by alpha - theta, we have to take the sum, this is equal to minimum R reflux ratio + 1. So alpha i is the relative volatility of component i with respect to some reference component, which is usually the heavy key or minimum is the minimum reflux ratio and x iD is the concentration of component i in the top product or distillate at minimum reflux condition.

And what is theta? Theta is the root of this equation, sigma alpha i x if alpha i - theta = 1 - q. So theta can be obtained by finding out the root of this equation. Here x if is the concentration of component i in the feed stream and q depends on the condition of the feed which is defined as heat required to vaporize one mole of feed divided by molar latent heat of the feed and you know that depending on condition of the feed q assumes different values.

For saturated liquid feed q =1, for saturated vapor feed q =0. If the feed is the liquid vapor mixture q will lie between 0 and 1. For subcooled liquid feed q is greater than 1 and for superheated vapor feed q is less than 0.
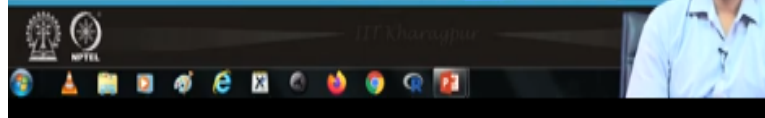
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Underwood Equation: Minimum Reflux Ratio

The relative volatilities in Underwood Equation are taken as constant. The geometric average of values estimated at the top and bottom temperatures should be used.

This requires an estimate of the top and bottom compositions. Though the compositions should strictly be those at minimum reflux, the values determined at total reflux, from the Fenske equation, can be used.

The value of θ must lie between the values of the relative volatility of the light and heavy keys, and is found by trial and error.

$$\sum \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 1 - q$$

$$\alpha_{HK} < \theta < \alpha_{LK}$$

The relative volatilities in underwood equations are taken as constant. The geometric average of values estimated at the top and bottom temperature should be used. This will require an estimation of the top and bottom compositions. Though the compositions should strictly be those at minimum reflux conditions as an approximation these values can be determined at total reflux using the Fenske equations.

Note that the value of theta which is a solution of this equation must lie between the values of the relative volatility of the light key and heavy key and this value of theta is found by trial and error method.

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Gilliland Correlation: Finite Reflux Ratio: Actual Trays

The Gilliland correlation provides an approximate relationship between number of stages and reflux ratio so that an optimal reflux ratio can be determined with a minimum of calculations.
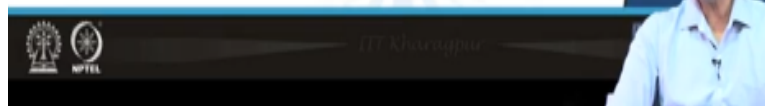
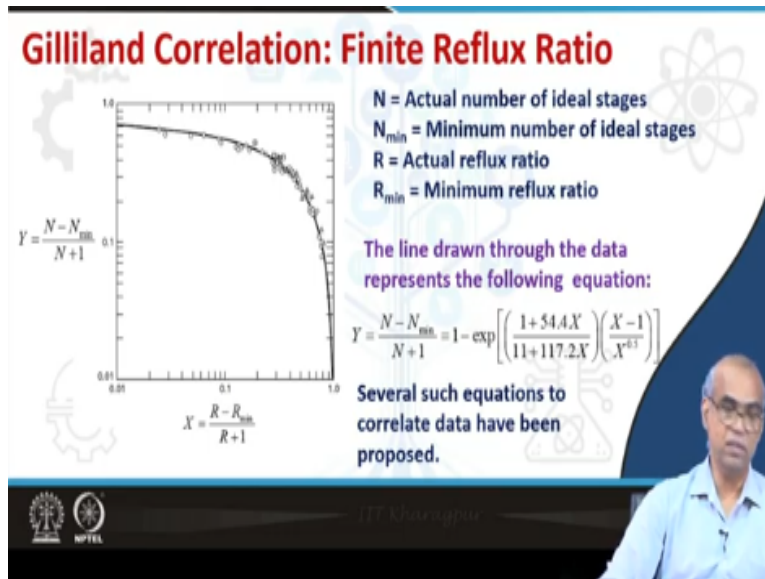Now after we have found out the minimum number of plates at total reflux condition using the Fenske equation and after finding the minimum reflux ratio using underwood equation will now find out the actual number of trays when you use finite reflux ratio by making use of Gilliland correlation. The Gilliland correlation provides an approximate relationship between number of stages and reflux ratio so that an optimal reflux ratio can be determined with a minimum of calculations.
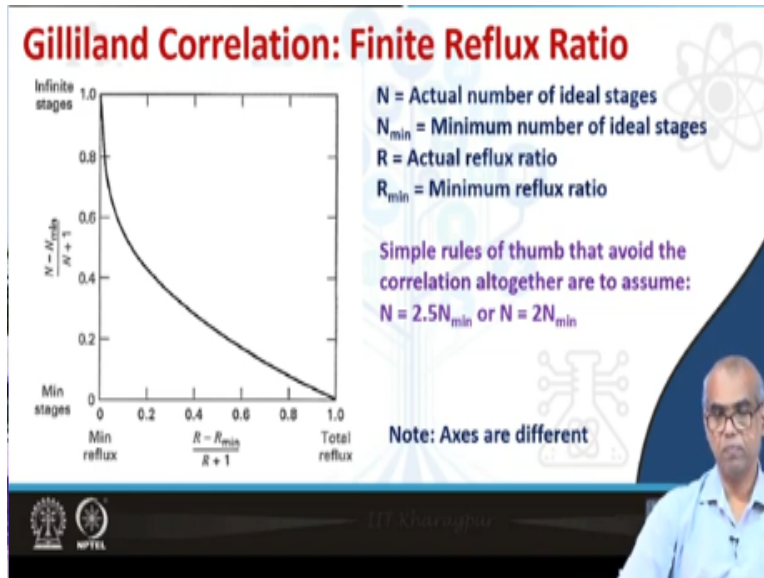
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Now the original correlation was presented in terms of graphs and then several atoms have been made to fit equations through this data. Now, if you look at the figure, the plot is between R minus R minimum by R + 1 versus N - N minimum by N + 1. Where N is the actual number of ideal stages, N minimum is the minimum number of ideal stages, R is actual reflux ratio and R minimum is minimum reflux ratio.

So, once we have found out the minimum number of ideal stages using the Fenske equation and we have found out the minimum reflux ratio using underwood equations then for various finite reflux ratio R, I can make use of this plot to find out the actual number of ideal trays required. So this is one equation that has been proposed in the literature which fits the data several such equations to correlate data have been proposed in the literature.

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Gilliland Correlation: Finite Reflux Ratio

N = Actual number of ideal stages
N_{min} = Minimum number of ideal stages
R = Actual reflux ratio
R_{min} = Minimum reflux ratio

Simple rules of thumb that avoid the correlation altogether are to assume:
$N = 2.5N_{min}$ or $N = 2N_{min}$

Note: Axes are different

This is the same plot but note that the axes are different. A simple thumb rule which will avoid the correlation altogether is that you can assume the actual number of plates is 2 times or 2.5 times the minimum number of plates, but that is the rule of thumb. We can always make use of this Gilliland correlation to get a better estimate.

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Feed Location:
➤ Use of Fenske Equation
➤ Use of Kirkbride Relation

Finally we see how to determine the feed location. This can be done using the Fenske equation, this can also be done using an empirical relation proposed by Kirkbride.

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Feed Location: Kirkbride Empirical Equation

The Kirkbride empirical equation provides a better approximation of the optimal feed-stage location:

$$\frac{N_R}{N_S} = \left[\left(\frac{x_{HK,F}}{x_{LK,F}}\right)\left(\frac{x_{LK,B}}{x_{HK,D}}\right)^2 \left(\frac{B}{D}\right)\right]^{0.206}$$

Total Number of Stages = $N_R + N_S$

N_R = number of stages above the feed, including any partial condenser
N_S = number of stages below the feed, including the reboiler
$x_{HK,F}$ = concentration of the heavy key in the feed
$x_{LK,F}$ = concentration of the light key in the feed
$x_{HK,D}$ = concentration of the heavy key in the top product
$x_{LK,B}$ = concentration of the light key if in the bottom product
D, B = Molar flow of distillate and bottoms, respectively

Gilliland correlation implicitly assumes that the stages are distributed optimally between the rectifying and stripping sections. The optimal feed stage can be located by assuming that the ratio of stage above the feed to stage below is the same as the ratio determined by applying the Fenske equation to the separate sections at total reflux conditions. So, the number of trays in the rectifying section divided by the number of trays in the stripping sections can be taken as number of trays in the rectified system under total reflux condition divided by number of trays in the stripping section under total reflux condition which can be obtained by the Fenske equation.

So this equation can be used, note that the total number of stages will be the number of stages in the rectifying sections plus number of stages in the stripping section, between these there will be the feed tray. However, a better approximation can be obtained by making use of an empirical equation proposed by Kirkbride and this is the empirical correlation, which is expressed in terms of concentrations of the heavy key in the feed, concentration of light in the feed, concentration of the light key in the bottom, concentration of heavy key in the bottom, bottom flow, distillate flow both are molar flow or bottom and molar flow of distillate.

So this gives me the ratio of the number of stages in the rectifying sections; that means the number of stages above the feed including partial condenser if N R and N S which represents number of stages in the stripping that means below the feed including the reboiler. So, we will better use this empirical correlation for determining feed location.

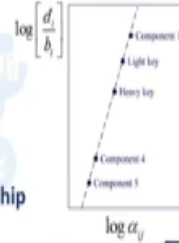Now finally we will talk about how to determine the distribution of non-key components. It can be done graphically using the Fenske equation. Note the Fenske equation in this form of molar flow rates of distillate and bottoms, you can take logs and can write this way. Note that this can be written as log di by bi equal to A + C log alpha i. The parameters A and C can be obtained by applying the relationship to the light key and heavy key components.

So I apply this relationship for light key and heavy key components and then we can find out the parameters A and C. Once we have found out the parameters A and C, the distribution of other components can be readily obtained by plotting the distribution of the keys against the relative volatility on log-log paper and drawing a straight line through these points as shown in this figure here. So this is how we can find out by making use of the Fenske equations graphically the distribution of non key components.

With this we stop our discussion here and in the next class, we will see an example of this FUG; Fenske key Underwood Gilliland shortcut method for design or multi component distillation column.