

Plant Design and Economics
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Lecture No -39

Design of Multi-component Distillation Column: Short Cut Method - Example

Welcome to lecture 39 of plant design and economics, in our previous lecture we have discussed Fenske-Underwood -Gilliland method as a shortcut method for design of multi component distillation system. So today we first briefly review whatever we have learnt in my previous class, and then we will take an example to demonstrate the application of the method.

(Refer Slide Time: 00:40)

Page: 2 / 2

Fenske-Underwood-Gilliland Method: Steps

Step-1:
Using Fenske Equation, estimate the minimum number of equilibrium stages, N_{\min} (corresponding to total reflux or infinite reflux ratio), needed to separate the two key components.

Step-2:
Using Fenske Equation, estimate the distribution, d/b , of each nonkey component between distillate and bottoms at total reflux using the value of N_{\min} computed in Step 1, the b/d ratio for the heavy key, and the relative volatility between the nonkey and the heavy key, $\alpha_{NK,HK}$.

So in the first step we use Fenske equation, to estimate the minimum number of equilibrium stages. This corresponds to total reflux or infinite reflux ratio. That is needed to separate the two key components. Next using Fenske equation, we estimate the distribution of each non-key components between distillate and bottoms at total reflux conditions, that means we will use the minimum number of theoretical plates that we have obtained using Fenske equation in the first step.

We can also compute the b by d ratio meaning the molar bottom flow rate divided by molar distillate rate for the heavy key and the relative volatility between the non-key and the heavy key. Will talk about this step after next few slides. In our previous lecture we have talked about the

graphical method for computation of distribution of non-key components.

(Refer Slide Time: 02:17)

Page 2 / 2

Fenske-Underwood-Gilliland Method: Steps

Step-3:
Use Underwood Equations to estimate the minimum reflux ratio, R_{\min} (corresponding to an infinite number of equilibrium stages), needed to separate the two key components.

Step-4:
Estimation by the Gilliland correlation of the actual number of equilibrium stages, N , for a specified ratio of actual reflux ratio, R , to minimum reflux ratio, R_{\min} .

Step-5:
Use Fenske Equation or Kirbride Empirical Equation to estimate the feed-stage location.

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In the step 3, we use Underwood equations to estimate the minimum reflux ratio, which corresponds to an infinite number of equilibrium stages, that will be needed to separate the two key components. In the step 4, we estimate by Gilliland correlation of the actual number of equilibrium stages for a specified ratio of reflux ratio R to minimum reflux ratio R_{\min} . So once we specify R by R_{\min} where R is the actual difference ratio and R_{\min} is the minimum reflex ratio that you have already obtained using underwood equation.

We can now make use of Gilliland correlation to find out the actual number of equilibrium stages. In the step 5, we have to find out the feed location for that we can make use of Fenske equation or we can also make use of Kirbride empirical equation.

(Refer Slide Time: 03:39)

Page: 6 / 6

Distribution of Non-key Components

From Fenske Equation:

$$\frac{d_i}{d_j} = \alpha_{ij}^{N_{\text{min}}} \frac{b_i}{b_j}$$

Combine with overall component balance: $f_i = d_i + b_i$

$$d_i = \frac{\alpha_{ij}^{N_{\text{min}}} f_i \left(\frac{d_j}{b_j}\right)}{1 + \alpha_{ij}^{N_{\text{min}}} \left(\frac{d_j}{b_j}\right)}$$

$$b_i = \frac{f_i}{1 + \alpha_{ij}^{N_{\text{min}}} \left(\frac{d_j}{b_j}\right)}$$

$$D = \sum_i d_i \quad B = \sum_i b_i$$

$d_i = x_{Di} D$
 $\Rightarrow x_{Di} = \frac{d_i}{D}$

Now the distribution of non-key components, we have seen how using Fenske equation we can find out the distribution of non-key components graphically. In our previous lecture we can also combine these equation with overall material balance around the distillation column and come up with an analytical expression for this ratio of distlet flow and the bottom slope. Note that, so this represents the overall component balance.

So if you combine this and the Fenske equation which has been written in d by b form. We can obtain by combining these two equations, the molar distillate flow as well as the molar bottom flow. Note that d i represents the molar distlet flow of component i. Similarly b i will represent molar bottom flow in the component i. So sum of d i will give me the total distillate flow and sum of b i will give me the total bottom flow.

So we can write d i is x d i into d. So the composition of ith component in the distillate can be found out as d i divided by d. Similarly we can also find for the bottoms.

(Refer Slide Time: 06:17)

The image shows a presentation slide with a blue background and white text. The title is 'Fenske-Underwood-Gilliland Method: Limitations' in red. The text describes the method's utility for initial estimates and its limitations for non-ideal mixtures. A speaker, a man in a pink shirt, is visible in the bottom right corner. The slide also features logos for IIT Kharagpur and NPTEL.

Page 7/7

Fenske-Underwood-Gilliland Method: Limitations

For ordinary distillation of a single feed to give only distillate and bottoms products, the FUG method is useful for making an initial estimate of the reflux ratio, the number of equilibrium stages, and the location of the feed stage.

The method is quite accurate for ideal mixtures of a narrow-boiling range. However, for nonideal mixtures, particularly those that form azeotropes, and for wide-boiling feeds, the FUG method can be quite inaccurate.

Therefore, before applying the method, the vapour-liquid equilibrium of the feed should be carefully examined for the magnitude of liquid-phase activity coefficients and the possibility of azeotropes over the range of possible compositions.

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Now before we take an example, let us now consider the limitations of the Fenske-Underwood-Gilliland method. For ordinary distillation of a single feed to give only distillate and bottoms product the Fenske-Underwood-Gilliland and method is useful for making an initial estimate of the reflux ratio, the number of equilibrium stages and the location of the feed stage. The method will be quite accurate for ideal mixtures of a narrow boiling range.

However for non-ideal mixtures particularly those that form azeotropes and for wide boiling feeds the Fenske-Underwood-Gilliland method can be quite inaccurate. So we should have an idea about the non ideality of the liquid mixture. To understand the applicability of the method or how much error that can be involved with the calculation. So before applying the method the vapor liquid equilibrium of the feed should be carefully examine.

For the magnitude of liquid phase activity coefficients and the possibility of azeotropes over the range of possible compositions. Note that the activity coefficients in the liquid phase will give us an idea about the deviation from the non-ideality. So there can be deviation positive deviation from Raoult's law, there can be negative deviation of Raoult's law. For example, if there can be positive deviations, you can get in minimum boiling as your term mixture.

So we should carefully look at the vehicle we have a liquid equilibrium data and look at the magnitude of the activity coefficients of the liquid phase. So that we can understand the

applicability of the method.

(Refer Slide Time: 08:41)

Fenske-Underwood-Gilliland Method: Example

Estimate the number of ideal stages needed in the butane-pentane splitter defined by the compositions given in the table below. The column will operate at a pressure of 8.3 bar. The feed is at its boiling point.

	Feed (<i>f</i>)	Tops (<i>d</i>)	Bottoms (<i>b</i>)
Propane, C ₃	5	5	0
i-Butane, iC ₄	15	15	0
n-Butane, nC ₄	25	24	1
i-Pentane, iC ₅	20	1	19
n-Pentane, nC ₅	35	0	35
	100	45	55 kmol

Relative Volatilities are computed as:

$$\alpha_i = \frac{K_i}{K_{HK}}$$

Component	α_i
C ₃	5
iC ₄	2.6
nC ₄ (LK)	2.0
iC ₅ (HK)	1.0
nC ₅	0.85

Now, let us take an example, estimate the number of ideal stages needed in the butane-pentane splitter defined by the compositions given in the table shown. The column will operate at a pressure of 8.3 bar, the feed is at its boiling point. So the value of that q is equal to 1. Now look at the data so Propane, iso-Butane, n-Butane, iso-Pentane and n-Pentane and what we want is a split between butane and pentane.

So I want to split here so my light key and heavy key components are this. So what we have need to do is we have to find the relative volatilities. So relative volatilities can be computed with help of the K values. So corresponding to with or with respect to the K value of heavy key, we compute the relative volatilities for all the components using α_i equal to K_i by K of heavy key.

Note that the informations on K values may be obtained from literature or it can also be estimated from equation of states such as say SRK equations. So you have obtained, let us say the alpha values so there are already arranged in the decreasing order of relative volatility and I want to split between butane and pentane. So my light key is n-Pentane and my heavy key is iso-Pentane.

(Refer Slide Time: 11:38)

Page: 11 / 11

Fenske-Underwood-Gilliland Method: Example

Distribution of components:

	α_i	f_i	d_i	b_i
C ₃	5	5	5	0
iC ₄	2.6	15	14.9	0.1
nC ₄ (LK)	2.0	25	24	1
iC ₅ (HK)	1	20	1	19
nC ₅	0.85	35	0.4	34.6
	100	D = 45.3	B = 54.7	

Find minimum number of stages using Fenske equation:

$$N_{\min} = \frac{\log \left[\frac{x_{LK}}{x_{HK}} \right]_{Distillate} \left(\frac{x_{HK}}{x_{LK}} \right)_{Bottoms}}{\log \alpha_{LK-HK}}$$

$$N_{\min} = \frac{\log \left[\left(\frac{24}{1} \right) \left(\frac{19}{1} \right) \right]}{\log (2)} = 8.8$$

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So the next stage will be to make use of the Fenske equation to estimate the minimum number of theoretical stages under total reflux plus condition. So we make use of the equation, so it involves the ratio of composition of light key to heavy key in the distillate. So, light key is 24 x light key and x heavy key is 1. Similarly x heavy key in the bottom by x light key in the bottom. So x heavy key is 19 and x light key is 1.

Now the value of alpha. So all these alphas are computed with respect to heavy key. So this alpha light key heavy key is 2. So if you do the computation, you get the minimum number of place as 8.8.

(Refer Slide Time: 13:53)

Page: 14 / 14

Fenske-Underwood-Gilliland Method: Example

Find minimum reflux ratio using Underwood equations.
As the feed is at its boiling point $q = 1$

Solve for θ : $\sum \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 1 - q = 0$

$x_{i,f}$	α_i	$\alpha_i x_{i,f}$	Try		
			$\theta = 1.5$	$\theta = 1.3$	$\theta = 1.35$
0.05	5	0.25	0.071	0.068	0.068
0.15	2.6	0.39	0.355	0.300	0.312
0.25	2.0	0.50	1.000	0.714	0.769
0.20	1	0.20	-0.400	-0.667	-0.571
0.35	0.85	0.30	-0.462	-0.667	-0.600
			$\Sigma = 0.564$	-0.252	0.022

close enough

$\theta = 1.35$

	α_i	f_i
C ₃	5	5
iC ₄	2.6	15
nC ₄	2.0	25
iC ₅	1.0	20
nC ₅	0.85	35

Dr. Kiranraj

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Next we have to find the minimum reflux ratio and we will use Underwood equations for this. We have been given that the feed is available at its boiling point so the value of the q is 1. So for value of q equal to 1. We first solve the value of theta. Note that the Underwood equations is basically stated in terms of two equations, we first have to solve this equation for the value of theta.

So theta is obtainable from the solutions of this equation. Now we need to compute $X_i f_i$, alpha has already given. We have to compute $X_i f_i$. So composition of component i in the feed. So how do you compute this quantity? This $X_i f_i$ is nothing but f_i divided by sigma f_i which is 100. So 5 by 100 is 0.05. 15 by 100 is 0.15 and so on and so forth. So we have tabulated the value of $X_i f_i$.

Now alpha is already given, so alpha $X_i f_i$, you multiply alpha $X_i f_i$ with corresponding $X_i f_i$ then with q equal to 1 we have to solve for theta. We try various values of theta and we see that with theta equal to 1.35, we are very close to this sum being 0. So theta equal to 1.35 can be considered as the solutions of this equations or root of this equation.

(Refer Slide Time: 17:03)

Fenske-Underwood-Gilliland Method: Example

Distribution of components:

	α_i	f_i	d_i	b_i
C_3	5	5	5	0
iC_4	2.6	15	14.9	0.1
nC_4 (LK)	2.0	25	24	1
iC_5 (HK)	1	20	1	19
nC_5	0.85	35	0.4	34.6
		100	$D = 45.3$	$B = 54.7$

Find minimum number of stages using Fenske equation:

$$N_{\min} = \frac{\log \left[\left(\frac{x_{LK}}{x_{HK}} \right)_{Distillate} \left(\frac{x_{HK}}{x_{LK}} \right)_{Bottoms} \right]}{\log \alpha_{LK-HK}}$$

$$N_{\min} = \frac{\log \left[\left(\frac{24}{1} \right) \left(\frac{19}{1} \right) \right]}{\log (2)} = 8.8$$

So now using theta equal to 1.35 will be able to compute minimum reflux ratio using Underwood equation. For this we need to compute $X_i d_i$ that means compositions of component i in the distillate. We have already found out the distribution of the components in our this table. Note that in the first table cell we find out using Fenske equations the minimum number of plates, we

find out the distribution of the components.

These distribution of the components now will use to find out the minimum reflux ratio. Note that these distribution of components have been used on the basis of total reflux condition. However it has been seen that this is an excellent starting case or excellence starting point even for the case where we want to find out the minimum reflux, minimum we want to find out the minimum reflux ratio.

(Refer Slide Time: 18:40)

Fenske-Underwood-Gilliland Method: Example
 Find minimum reflux ratio using Underwood equations (Cont'd):

Now use $\theta = 1.35$ and $\sum \frac{\alpha_i x_{i,D}}{\alpha_i - \theta} = R_{\min} + 1$

$x_{i,d}$	α_i	$\alpha_i x_{i,d}$	$\alpha_i x_{i,d} / (\alpha_i - \theta)$
0.11	5	0.55	0.15
0.33	2.6	0.86	0.69
0.53	2.0	1.08	1.66
0.02	1	0.02	-0.06
0.01	0.85	0.01	-0.02
			$\Sigma = 2.42$

	α_i	f_i	d_i	b_i
C_3	5	5	5	0
iC_4	2.6	15	14.9	0.1
nC_4 (LK)	2.0	25	24	1
iC_5 (HK)	1	20	1	19
nC_5	0.85	35	0.4	34.6
	100	$D = 45.3$	$B = 54.7$	

$R_{\min} + 1 = 2.42$
 $\Rightarrow R_{\min} = 1.42$

So we have to now compute the $X_{i,d}$, so this we can compute as we said that $x_{i,d}$ is d_i divided by D . Note that the d is sum of d_i and b is sum of b_i . So this can be obtained as 5 by 45.3, so say 5 by 45, which is 1 by 9 so close to 0.11. Next 0.33 is obtained as 14.9 divided by 45.3. So you can roughly say 15 by 45 is 1 by 3, which is 0.33 so on and so forth. So this way I find out $X_{i,d}$ that means the concentrations of component i in the distillate.

Alpha as are known find out the product $\alpha_i X_{i,d}$ and then find out this sum, which is obtained as 2.42. So in the right hand side, we have 1 plus or minimum which is equal to 2.42, so minimum reflux ratio is obtained as 1.42. So this is what we obtained using Underwood equations the minimum reflux ratio equal to 1.42.

(Refer Slide Time: 21:08)

Page: 20 / 20

Fenske-Underwood-Gilliland Method: Example

Find actual number of trays and finite reflux ratio using Gilliland Correlation:

$Y = \frac{N - N_{\min}}{N + 1}$

$X = \frac{R - R_{\min}}{R + 1}$

Consider: $R = 2.0$ $R_{\min} = 1.42$, $N_{\min} = 8.8$

$$X = \frac{R - R_{\min}}{R + 1} = \frac{2 - 1.42}{2 + 1} = 0.193$$

From Graph: $Y = \frac{N - N_{\min}}{N + 1} = 0.40 \Rightarrow N = 15.3$

R	2	3	4	5	6
N	15.3	12	10.7	10.4	10

For $R > 4$, there is little change in the number of stages required. R_{optimum} will be near this value.

Next let us use Gilliland correlation to find out the actual number of trays for finite reflux ratio. Now let us consider say R equal to 2 you can consider various values of R by R minimum. Let us consider R equal to 2, we have already obtained minimum reflux ratio as 1.42 and minimum number of theoretical stages as Fenske equation as 8.8. Now Gilliland correlations is a plot between $R - R_{\min}$ by $R + 1$ and $N - N_{\min}$ by $N + 1$.

So you compute $R - R_{\min}$ by $R + 1$ as 0.193, so corresponding to say close to 0.2 which is this we obtain 0.234 about 0.4. Approximately you can find out this more accurately of course. So from the graph we find $N - N_{\min}$ by $N + 1$ say as point 4. With the value of N_{\min} as 8.8 we get N equal to about 15.3. Now we can repeat this computation for various values of reflux ratio R.

For example with reflux ratio 3, I get the actual number of stages as 12, with R equal to 4 I get N equal to 10.7 and so on and so forth. What you can see that when the plus ratio is greater than 4 there is little change in the number of stages that are required and are optimum, the optimum reflux ratio will be near this value 3, 4 like that. So now we have obtained minimum number of stages, then we obtain the minimum reflux ratio using Underwood equation and now we obtained the actual number of stages for various values of reflux ratio using Gilliland method.

(Refer Slide Time: 24:21)

Page: 24 / 24

Fenske-Underwood-Gilliland Method: Example

Estimate the Feed location using Kirkbride
Empirical Relation:

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

$$x_{b,LK} = \frac{1}{54.7} = 0.018$$

$$x_{d,HK} = \frac{1}{45.3} = 0.022$$

$$\log \left(\frac{N_r}{N_s} \right) = 0.206 \log \left[\frac{54.7}{45.3} \left(\frac{0.20}{0.25} \right) \left(\frac{0.018}{0.022} \right)^2 \right]$$

$$\log \left(\frac{N_r}{N_s} \right) = 0.206 \log(0.65)$$

$$\frac{N_r}{N_s} = 0.91$$

	α_i	f_i	d_i	b_i	$x_{i,f}$
C_3	5	5	5	0	0.05
C_4	2.6	15	14.9	0.1	0.15
nC_4 (LK)	2.0	25	24	1	0.25
iC_5 (HK)	1	20	1	19	0.20
nC_5	0.85	35	0.4	34.6	0.35
		100	$D = 45.3$	$B = 54.7$	

Now we will find out the feed location and for this let us use Kirkbride empirical relation, which is more popular than the Fenske method of determination of feed location. And we know that, the empirical correlation for determination of feed location is given. Note that this will require the concentrations of heavy key, light key in the feed. Concentration of the light key in the bottoms and concentration of the heavy key in the bottoms as well as distillate flow and molar distillate flow and molar bottom flow.

So we have all these values, now we are in a position to find out the ratio of the number of ideal stages in the rectifying section to the number of ideal stages in the stripping section, N_r by N_s . N_r rectifying section divided by N_s stripping section. So let us now compute, we need the concentration of light key in the bottoms. The concentration of the light key in the bottoms can be obtained as 1 divided by 54.7 which is 0.018.

Similarly concentration of heavy key in the distillate which can be obtained as 1 divided by 45.3, which is 0.022. Other values $B = 54.7$, $D = 45.3$, then concentration of heavy key in the feed which is obtained as 0.20 and concentrations of light key in the feed which is obtained as 0.25. So all the values once you put in the equation you can find out the ratio of number of stages in the rectifying section, to the number of stages in the stripping as 0.91.

(Refer Slide Time: 28:07)

Page 25 / 25

Fenske-Underwood-Gilliland Method: Example

Estimate the Feed location using Kirkbride

Empirical Relation:

$$x_{b,LK} = \frac{1}{54.7} = 0.018$$

$$x_{d,HK} = \frac{1}{45.3} = 0.022$$

$$\log\left(\frac{N_r}{N_s}\right) = 0.206 \log\left[\frac{54.7}{45.3} \left(\frac{0.20}{0.25}\right) \left(\frac{0.018}{0.022}\right)^2\right]$$

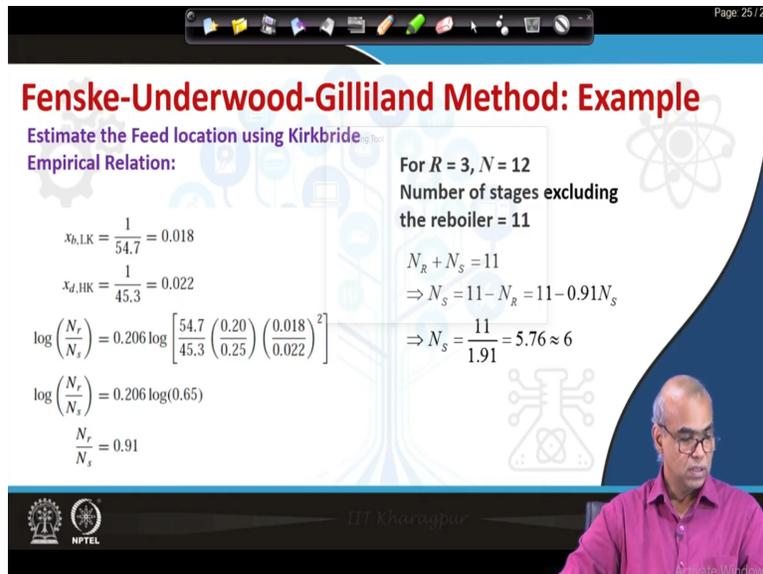
$$\log\left(\frac{N_r}{N_s}\right) = 0.206 \log(0.65)$$

$$\frac{N_r}{N_s} = 0.91$$

For $R = 3$, $N = 12$
Number of stages excluding the reboiler = 11

$$N_r + N_s = 11$$

$$\Rightarrow N_s = 11 - N_r = 11 - 0.91N_s$$

$$\Rightarrow N_s = \frac{11}{1.91} = 5.76 \approx 6$$


Now let us do a computation let us consider reflux ratio R equal to 3, the actual reflux ratio R equal to 3. For this value we have seen that the actual number of stages is 12, so number of stages excluding the reboiler is 11, because N equal to 12 includes reboiler, so number of stages excluding the reboiler is 11. Note so $N_r + N_s$ is if I let 11 and we know N_r by N_s equal to 0.91, so we can find out N_s .

So N_s is $11 - N_r$, N_r is nothing but 0.91 into N_s . See you solve this for N_s and you get the value of N_s as about 6. So then N_r can also be obtained as 0.91 into 6. So this way you can find out the N_r and N_s . So the number of stages in the rectifying section and the number of stages in the stripping sections. So this gives you the feed location which separates the rectifying section and the stripping section.

So the application of the Fenske underwood Gilliland method to determine the minimum number of stages the minimum reflux ratio and finally which is the main objective is to find out the actual number of stages the feed location and the corresponding reflux requirement. All this can be found out using this shortcut method.

(Refer Slide Time: 30:23)

Page 26 / 26

AspenPlus: Module for Distillation Column Design

AspenPlus:

- > Shortcut methods: DSTWU
- > Rigorous method: RADFRAC

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These days in almost all cases the process simulators are used for design or multi component distillation column. Almost all process simulators has also a module which implements the shortcut method. For example aspen plus the module DSTWU implements this shortcut method whereas the rigorous method which involves the detail solutions of those mesh equations material balance, heat balance equilibrium relation and the summation.

So those involves solutions of those mesh equations forms the basis of the rigorous methods and the rigorous method is available in the module RADFRAC, whereas DSTWU is available in the aspen plus and this implements the shortcut method. So what we learned in these lecture is how to compute the actual number of stages corresponding reflux conditions, F sector feed locations for a multi component distillation column using shortcut method.

Now there are other aspects of distillation design column as well you have to find out the height which can be obtained from the knowledge of number of the trays and the tray spacing. The diameter of the distillation column the internals the diameters typically depends on the wave of flow rate, which you can compute using several correlations and using the concept of no flooding in the distillation column. With this we stop our discussion today here.