Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 32
FUG method of stage calculations

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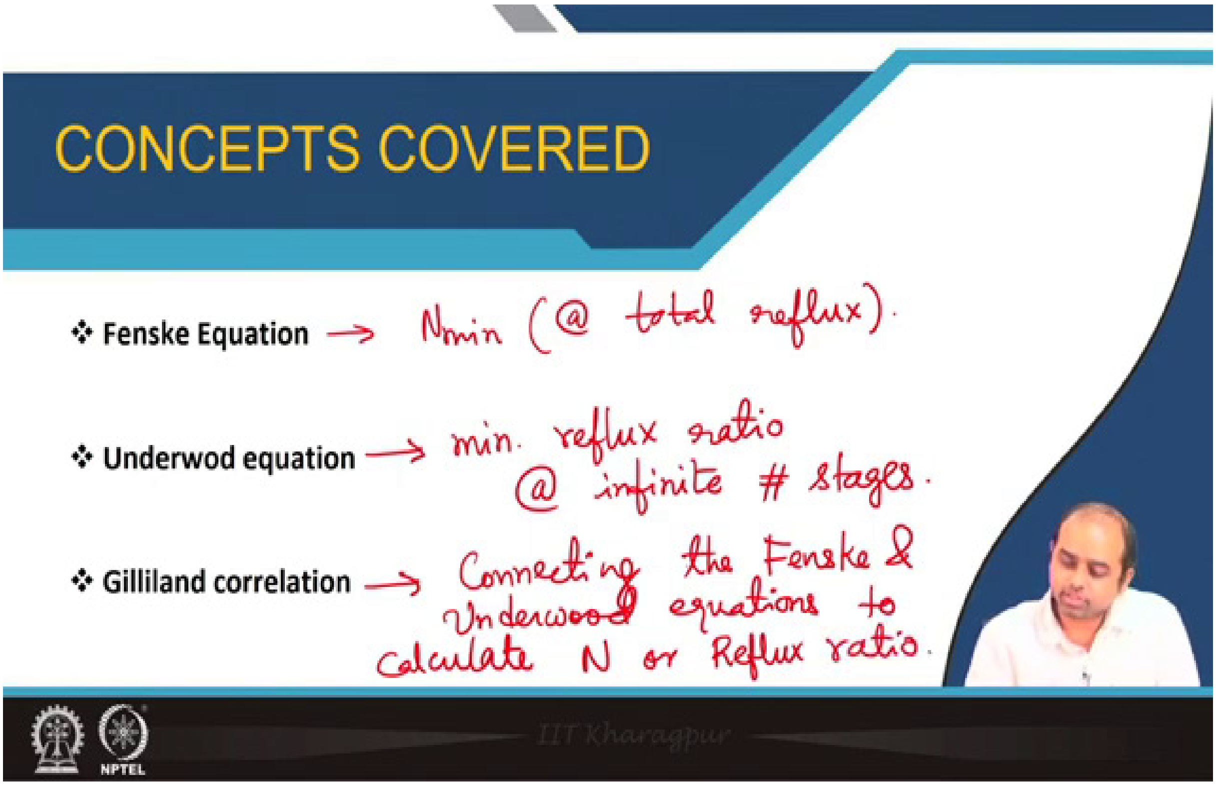

CONCEPTS COVERED

- Fenske Equation → N_{min} (@ total reflux).
- Underwod equation → min. reflux ratio @ infinite # stages.
- Gilliland correlation → Connecting the Fenske & Underwood equations to calculate N or Reflux ratio.

Hello everyone in this lecture we are going to talk about the shortcut or the approximate method of calculating the number of stages and the optimum reflux ratio in this process. So, this is something known as based on three persons, the Fenske, Underwood, and the Gilliland equation. So, the Fenske equation talks about the minimum number of the stages, the Underwood equation talks about the minimum reflux condition and to using this together you have the Gilliland correlation which helps you determine for the given number of stages or given reflux ratio what would be the number of stages or alternatively what would be the number of, what would be the reflux amount.

So, all of that when you, so Fenske equation is for the case of minimum number of stages at the condition of total reflux and Underwood equation tells you minimum reflux ratio at infinite number of stages. So, these are the two possible extremes actually. So, this is Gilliland correlation is connecting these above two, connecting the Fenske and Underwood equations to calculate the number of stage or the reflux ratio. So, first we will talk about the Fenske equation then the Underwood equation and finally the Gilliland correlation.

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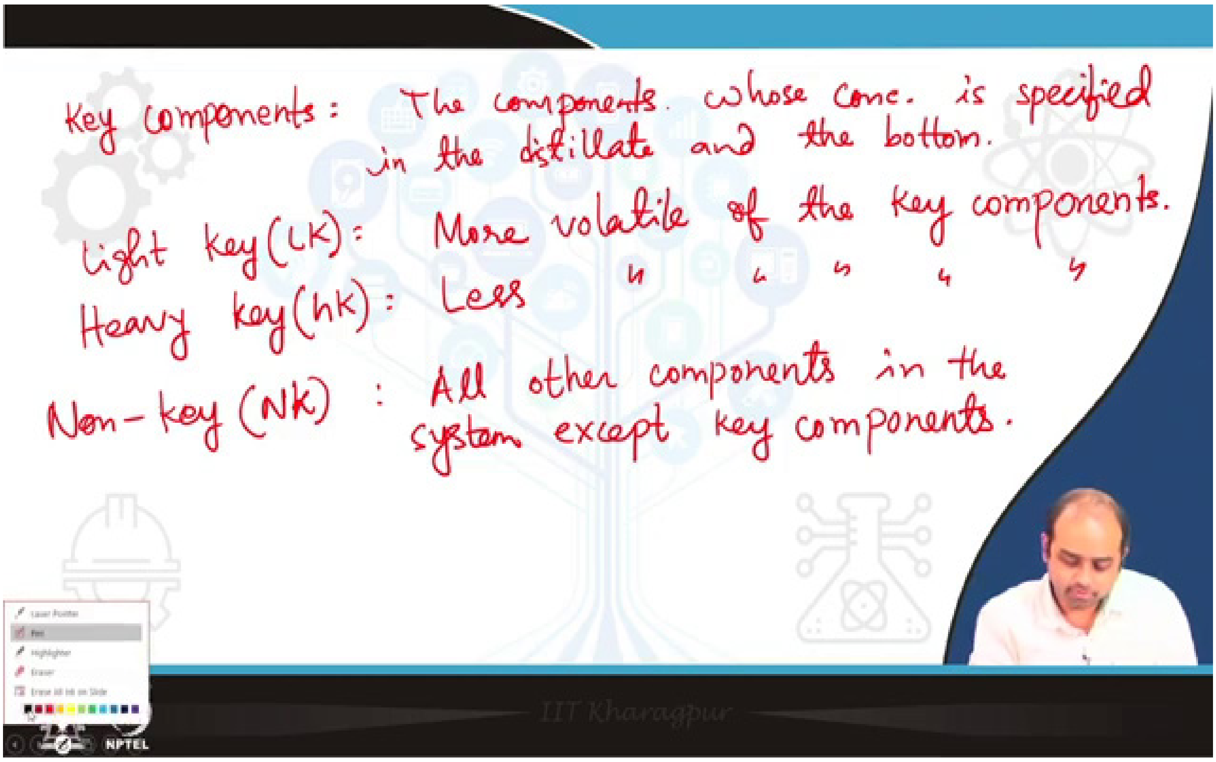
Key components : The components whose Conc. is specified in the distillate and the bottom.

Light key (LK) : More volatile of the key components.

Heavy key (HK) : Less " " " " "

Non-key (NK) : All other components in the system except key components.

Before we go ahead, I also like you to highlight or give you some information regarding what we min by key components. So, the components whose concentration is specified in the distillate and the bottom, so these are called the key components. Next is known as something known as the light key and the heavy key. So, light key is more volatile of the key components and heavy key is the less volatile of the key components. So, there is something also known as non-key component, so this is all other components in the system except key components. Now, let us look into the situation for the Fenske equation.

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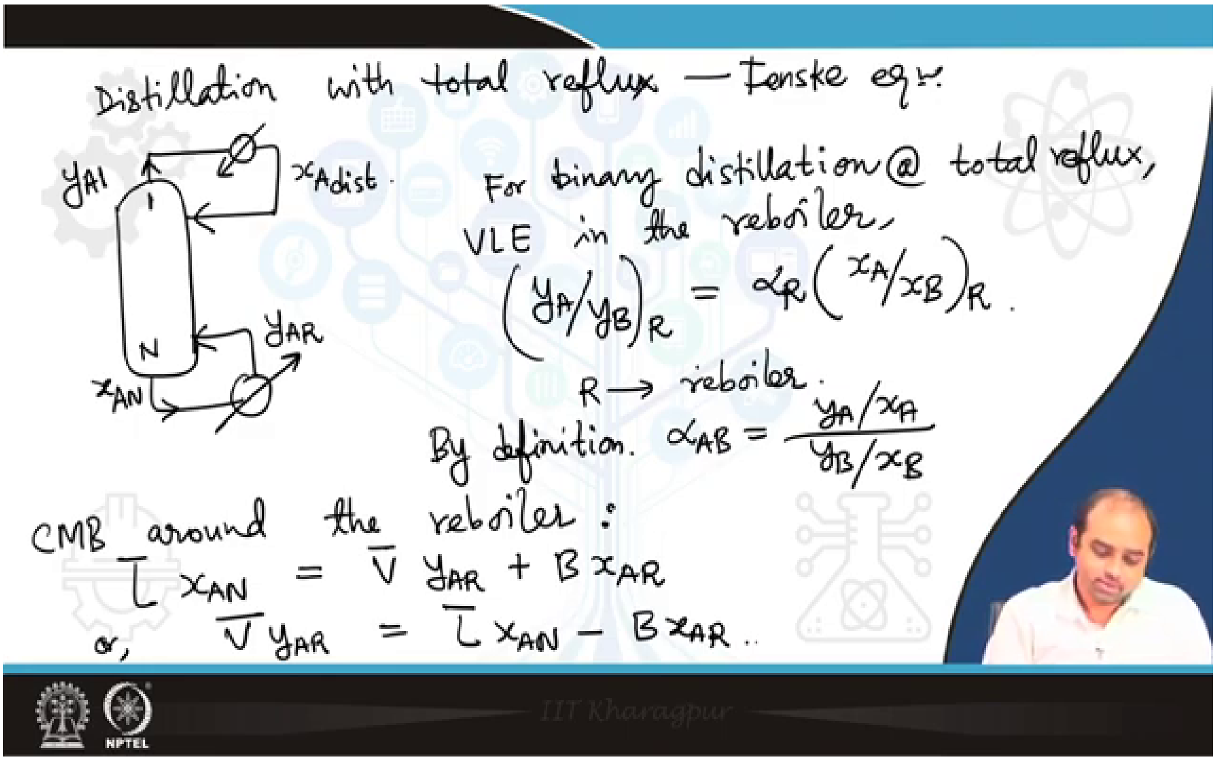

Distillation with total reflux — Fenske eqn.

For binary distillation @ total reflux,
VLE in the reboiler,

$$\left(y_A/y_B\right)_R = \alpha_R\left(x_A/x_B\right)_R.$$

R → reboiler.

By definition. $\alpha_{AB} = \dfrac{y_A/x_A}{y_B/x_B}$

CMB around the reboiler:

$$\bar{L}\,x_{AN} = \bar{V}\,y_{AR} + B\,x_{AR}$$

or, $\bar{V}\,y_{AR} = \bar{L}\,x_{AN} - B\,x_{AR}$..

So, distillation with total reflux. So, let us say you have the distillation column like this and you have the reboiler, you have total N number of stages excluding the reboiler and again you have the total condenser. So, the total, the top vapor fraction is let us say is written by like this I mean y B i and whatever number of components that we are having, similarly, the liquid phase can be written known as x dist, not confusing, let us write only A y i, y A i, similarly the bottom is x A N, it is not A i, it is A 1, the top tray composition, a top phase vapor and all.

And for the reboiler let us write down as y A R. So, x A N is the liquid phase composition that is going into the reboiler from the last stage, y A 1 is the top vapor composition that is going into the total condenser. So, for binary component, for binary distillation this is true I mean the Fenske equation also holds for distillation at total reflux. VLE Vapor Liquid Equilibrium in the reboiler tells you that y A by y B at the reboiler is equal to alpha is the relative volatility at the reboiler, this is true for the reboiler, R denotes the reboiler.

And this is true because from definition we know that alpha A B is y A by x A divided by y B by x B, this is something by definition we know. So, now making a component mass balance around the reboiler and then we try to use those equation to substitute y A and y B and all those things. So, L x A N, I write L as L bar because this is the stripping part V bar y A R plus B into x A R this is around the reboiler. So, or I can write V y A R is equal to L bar x A

N minus B x A R so this is if I am trying to make a mass balance or component mass balance around the reboiler.

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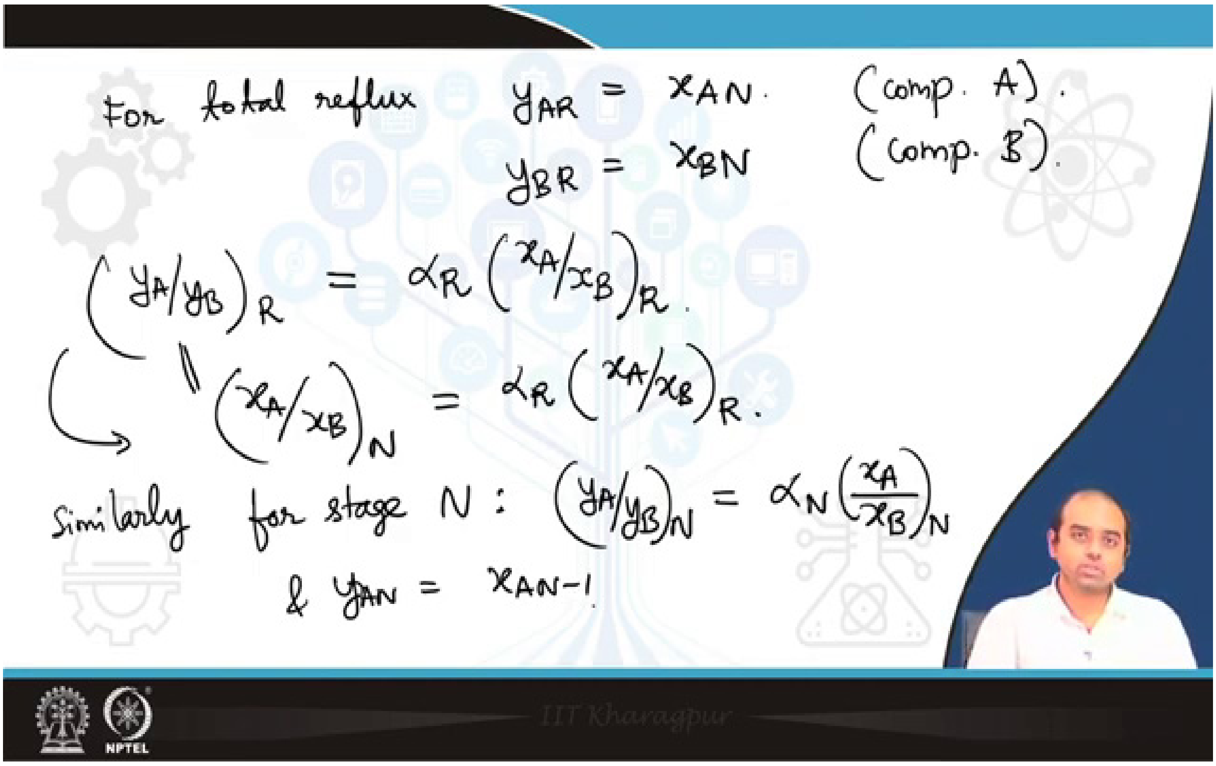


For total reflux $y_{AR} = x_{AN}$. (comp. A).

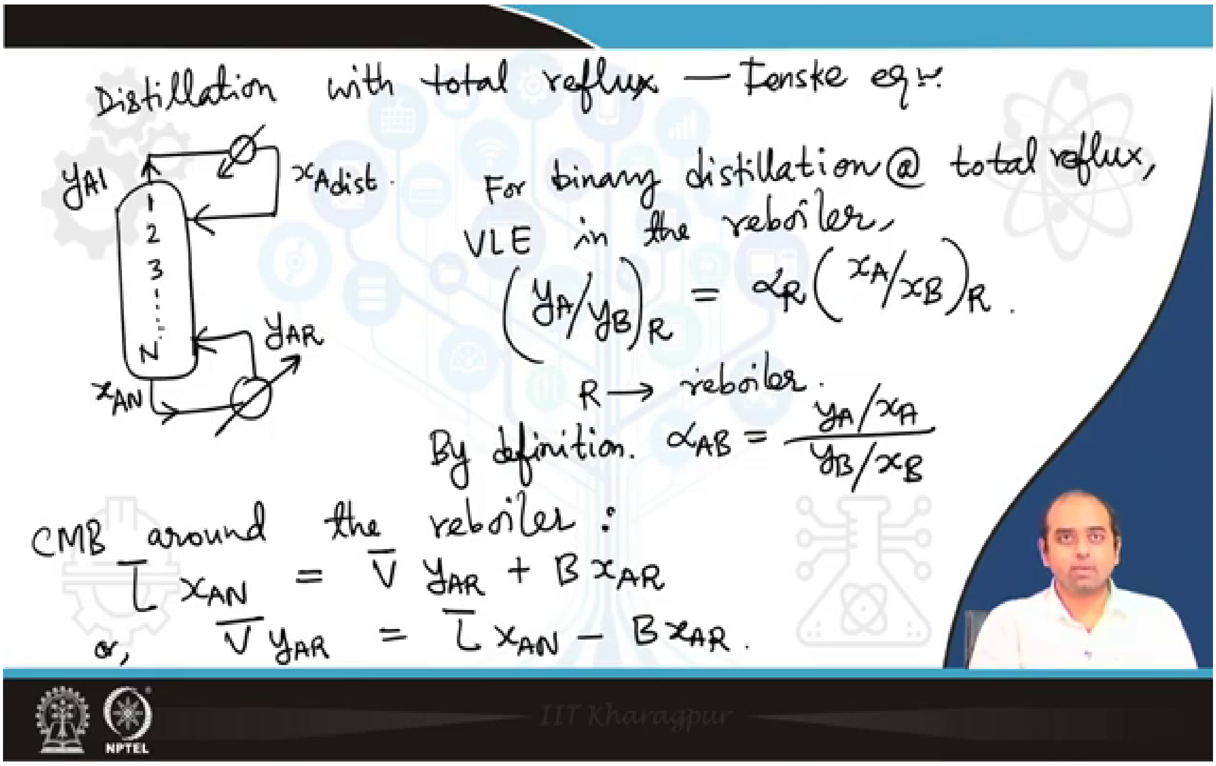
$y_{BR} = x_{BN}$ (Comp. B).

$$\left(y_A/y_B\right)_R = \alpha_R \left(x_A/x_B\right)_R .$$

$$\left(x_A/x_B\right)_N = \alpha_R \left(x_A/x_B\right)_R .$$

Similarly for stage N: $\left(y_A/y_B\right)_N = \alpha_N \left(\frac{x_A}{x_B}\right)_N$

& $y_{AN} = x_{AN-1}$



Distillation with total reflux — Fenske eqn.

For binary distillation @ total reflux, VLE in the reboiler,

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R → reboiler.

By definition. $\alpha_{AB} = \dfrac{y_A/x_A}{y_B/x_B}$

CMB around the reboiler:

$$\bar{L}\, x_{AN} = \bar{V}\, y_{AR} + B\, x_{AR}$$

or, $\bar{V}\, y_{AR} = \bar{L}\, x_{AN} - B\, x_{AR}$.

So, for total reflux we got in the reboiler of course we have y A R is equal to x A N everything the mass or the mole fractions that is in the liquid state that is entering the reboiler is getting completely converted to the vapor part into the system and similarly this is for component A. Similarly, for component B you have y B R is equal to x B N, that is true.

Now, from here we can write so let us call this from these two equations, I mean using these two equations you can write y A by y B in the reboiler is equal, I mean this equation we already have. Now, this can be written down, I mean this equation can be written down as x A by x B N is equal to alpha r x A by x B at the reboiler. This is we are equating from the above equation y A R is equal to x A N.

Now, similarly for stage N, I can write y A by y B Nth stage is equal to alpha N x A by x B at the Nth stage this is possible from the equation of the relative volatility. And we have this y A N is equal to x A N minus 1, I mean I hope all of you know the type of nomenclature we make for the trays.

So, the liquid that is coming from the previous tray is getting vaporized and is becoming the vapor fraction is equivalent to the liquid composition from the previous tray. So, this relation always holds. So, I hope I should write down how the 1, 2, this stage numbering is done. So, if you have any particular stage, the vapor leaving I mean the vapor composition leaving from that stage is equivalent is equivalent to the liquid that is coming to that tray from the previous stage, that is how the numbering is done and that is why these relations hold. Similarly, it holds for B N also. Now, you can continue to do the same thing.

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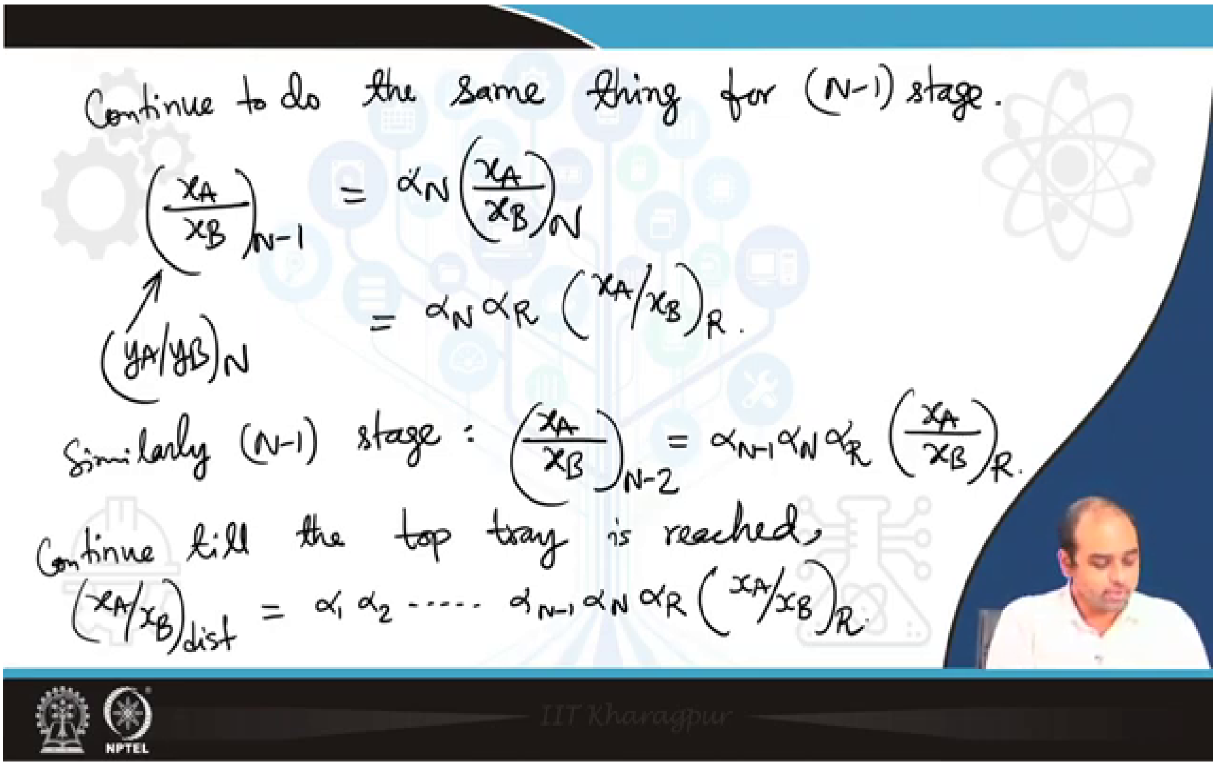

Continue to do the same thing for (N-1) stage.

$$\left(\frac{x_A}{x_B}\right)_{N-1} = \alpha_N \left(\frac{x_A}{x_B}\right)_N$$

$$(y_A/y_B)_N$$

$$= \alpha_N \alpha_R \left(x_A/x_B\right)_R .$$

Similarly (N-1) stage : $\left(\frac{x_A}{x_B}\right)_{N-2} = \alpha_{N-1}\alpha_N\alpha_R\left(\frac{x_A}{x_B}\right)_R .$

Continue till the top tray is reached,

$$(x_A/x_B)_{dist} = \alpha_1 \alpha_2 \cdots \alpha_{N-1}\alpha_N\alpha_R\left(x_A/x_B\right)_R .$$

So, we can continue to do the same thing for N minus 1 stage. So, we will get, what we will get? I mean this is something we can continue to do for any stage, not for N minus 1 stage, N minus 2, N minus 3 like that. So, what we are getting? So, from the N stage what we are getting x A by x B for the, this one we are getting for N stage, this is something we are getting and this we are actually equating as y A by y B N.

Now, on the right-hand side this can be written down as x N, alpha N alpha R x A by x B R. Similarly, I can continue this, I can continue this for N minus 1 and for any stage actually. So, for the N minus 1 stage we will get x A by x B as N minus 2 is equal to alpha N minus 1 alpha N alpha R, everything can be required to the reboiler. So, we can continue up to top, continue till the top tray is reached so we get x A by x B in the distillate is equal to alpha 1, alpha 2, dot, dot, dot alpha N minus 1, alpha N, alpha R it can be related to the reboiler.

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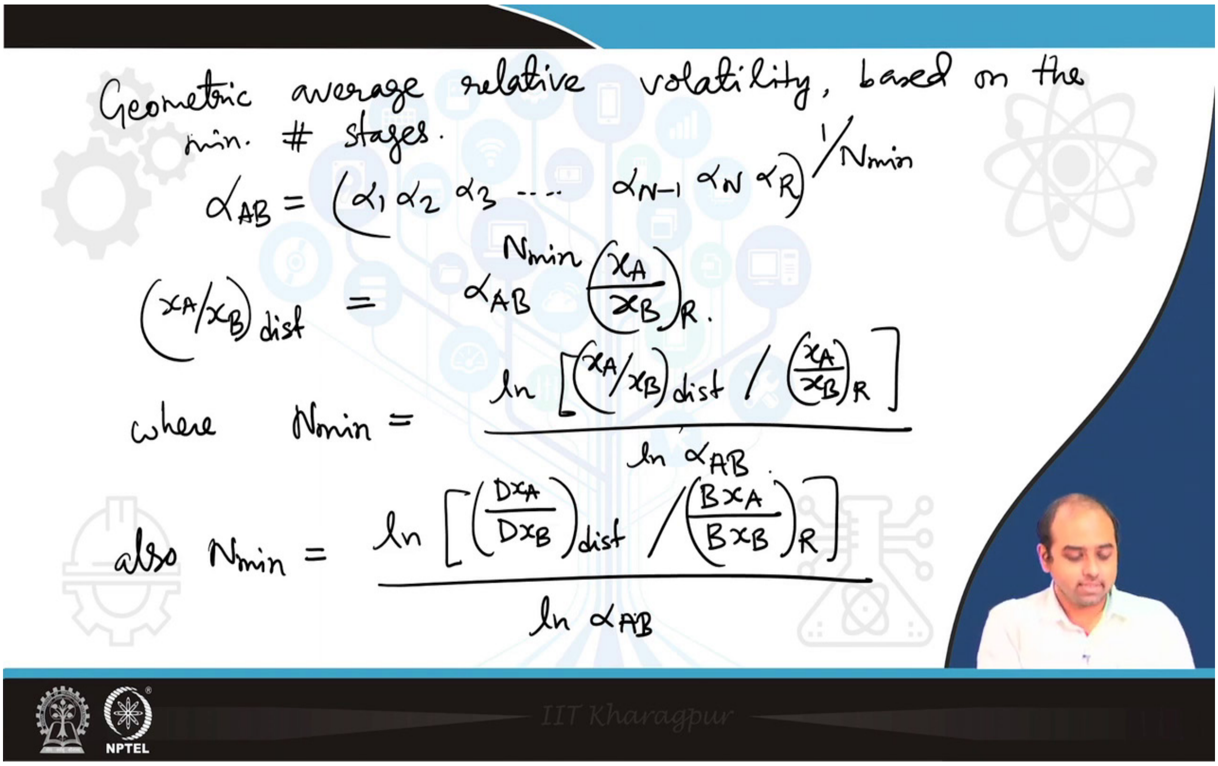

Geometric average relative volatility, based on the min. # stages.

$$\alpha_{AB} = (\alpha_1 \alpha_2 \alpha_3 \cdots \alpha_{N-1} \alpha_N \alpha_R)^{1/N_{min}}$$

$$(x_A/x_B)_{dist} = \alpha_{AB}^{N_{min}} \left(\frac{x_A}{x_B}\right)_R.$$

where $$N_{min} = \frac{\ln\left[(x_A/x_B)_{dist} \Big/ \left(\frac{x_A}{x_B}\right)_R\right]}{\ln \alpha_{AB}}.$$

also $$N_{min} = \frac{\ln\left[\left(\frac{Dx_A}{Dx_B}\right)_{dist} \Big/ \left(\frac{Bx_A}{Bx_B}\right)_R\right]}{\ln \alpha_{AB}}$$

So, if we try to define, if you try to define a sort of the geometric average, geometric average relative volatility based on the minimum number of stages something like alpha A B is equal to alpha 1 alpha 2 alpha 3 N minus 1 alpha N alpha R to the power 1 by N min so this is the geometric min based on the, for the minimum number of stages in this case.

So, we can write x A by x B in the distillation I min in the top fraction as alpha A B to the power N min, x A by x B at R so where N min can be written down as log of x A by x B distillation divided by x A by x B at r divided by ln alpha A B. You can also write this, you can also write, also write this N min as in terms of the fractional components or you can also write this as D x A by D x B, D is the distillate rate divided by B, B is the part of the reboiler, this is also possible. So, we you can write this N min based on the fractional recovery of the system that is also possible to write in this case. How? Let us also work that out.

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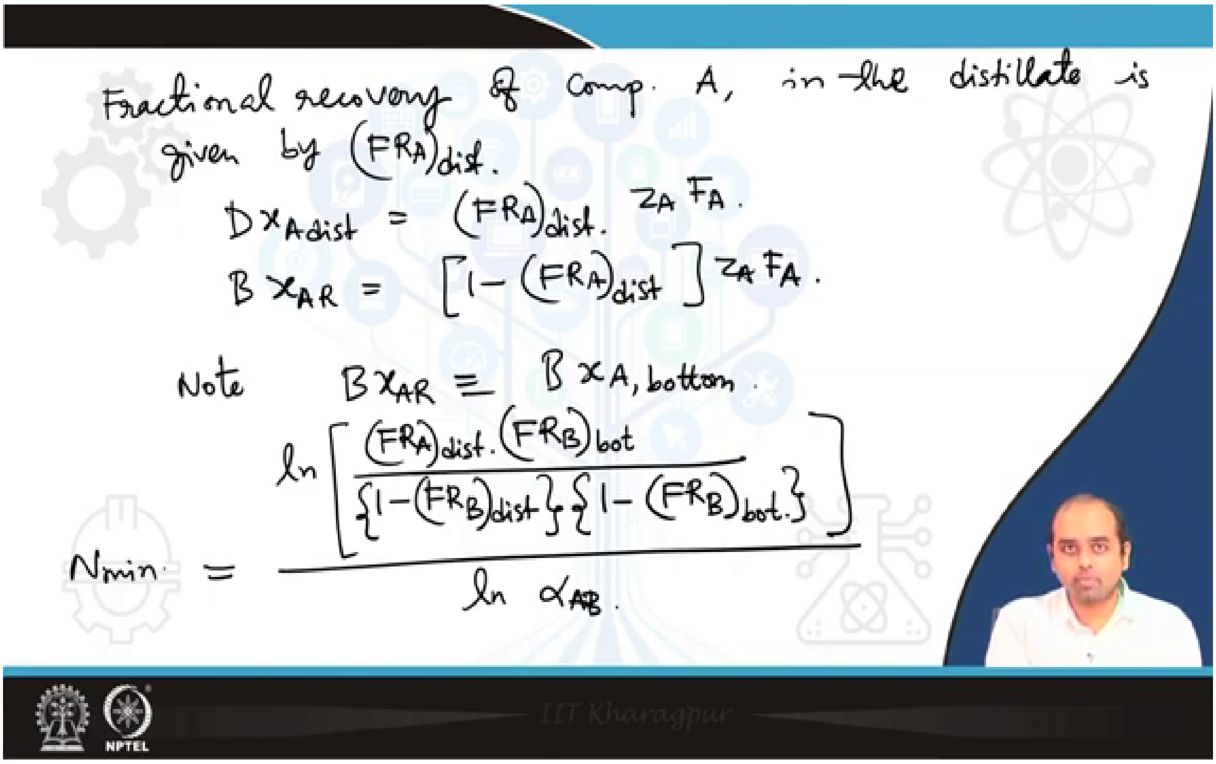

Fractional recovery of comp. A, in the distillate is given by $(FR_A)_{dist}$.

$$D x_{A dist} = (FR_A)_{dist} \cdot z_A F_A .$$

$$B x_{AR} = \left[1-(FR_A)_{dist}\right] z_A F_A .$$

Note $B x_{AR} = B x_{A, bottom}$.

$$N_{min} = \frac{\ln\left[\dfrac{(FR_A)_{dist} \cdot (FR_B)_{bot}}{\{1-(FR_B)_{dist}\}\{1-(FR_B)_{bot}\}}\right]}{\ln \alpha_{AB}} .$$

So, for the key components I can also write that the fractional recovery of component A, the key component A in the distillate is given by let us say F R A distillate. Then what do we get? I can write D x A distillate is equal to this is something I can write fractional recovery into Z A F A, similarly, I can also write B x A R is equal to 1 minus F R A, so F is the feed, molar feed flow rate and x A is the mole fraction of A in the feed.

And also, please note that B x A R is equal to B x A at the bottom. So, similarly, I can write the same equations for component B. So, if in that case I can rewrite my N min as F R A in the distillate then F R B in the bottom divided by 1 minus F R A distillate 1 minus F R A, sorry this is F R B, this is I think 1 minus B, F R B in the bottom divided by l n of alpha A B, this is the N minimum in terms of fractional recovery, F R B at the bottom is of course the fractional recovery of component B at the bottom. So, for binary system so this is for multi component systems and based on the key components we can write this equation.

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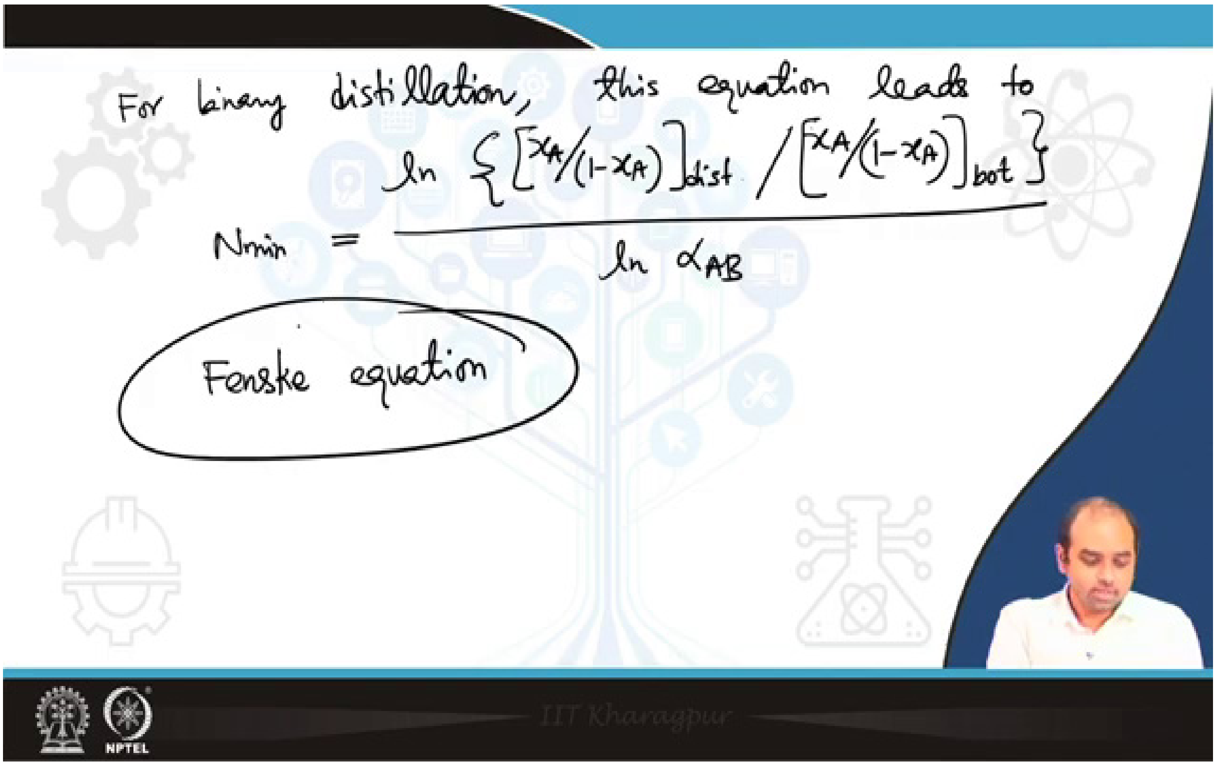

For binary distillation, this equation leads to

$$N_{min} = \frac{\ln \left\{ \left[x_A/(1-x_A) \right]_{dist} / \left[x_A/(1-x_A) \right]_{bot} \right\}}{\ln \alpha_{AB}}$$

Fenske equation

So, for binary equation this equation I min for binary distillation, this equation leads to as N minimum ln x A by 1 minus x A at the distillate divided by x A by 1 minus x A at the bottom. So, this is the N minimum so this is known as the Fenske equation. So, which were the number of trays or the minimum number of trays based on the total reflux condition can be estimated on the knowledge of the, this relative volatility or some gross relative volatility of the mixture and provided the top and the bottom compositions of the key components are known. Now, let us now quickly move to the Underwood equations.

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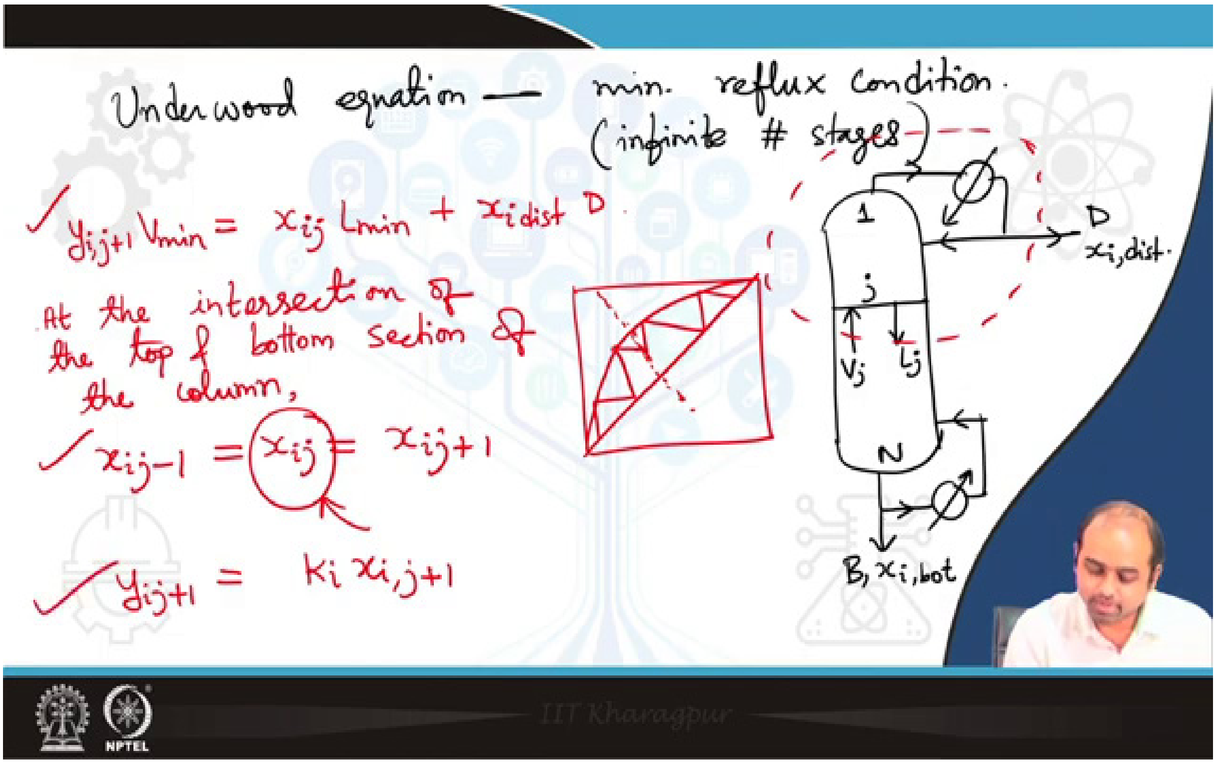

Underwood equation — min. reflux condition. (infinite # stages)

✓ $y_{ij+1} V_{min} = x_{ij} L_{min} + x_{idist} D$

At the intersection of the top & bottom section of the column,

✓ $x_{ij-1} = x_{ij} = x_{ij+1}$

✓ $y_{ij+1} = K_i x_{i,j+1}$

So, in the case of the Underwood equation which is applicable. So this Underwood equation is applicable for the minimum reflux condition and of course the natural consequence is that for minimum reflux you have infinite number of stages. So, again let us draw the simple distillation column and mark the streams, so always we have a total reboiler and here so this is stage 1, this is stage N, let us say arbitrary number of, as arbitrary stage j, so the vapor that is coming in is V and let us I mean V j and let us call this as L j and this D and x i distillate, the bottom part if you are taking out anything from the bottom we can call this as B x i bottom.

So, let us try to do a mass balance in enriching part. So, we try to write down a mass balance in the enriching part. So, we get y i j plus 1 V min is equal to x i j L min plus x i dist that is D, so this is for the enriching section you have the minimum flow rates of your liquid and the vapors and around the intersection of the top and the bottom operating line if you recall that graphical construction where you have you remember that Q line and then when you try to draw the stages when you try to draw the stages so this is something you are used to and familiar to doing.

So, then we had the Q line and at the Q line then we said the feed stage has to be passed, so at the intersection of, that is how we segregate as the top and the bottom section of this column. So, at the intersection of the top and the bottom section, intersection of the top and bottom part of the column, we have x i j minus 1 so please note j represents the stage and i represent the component as this, so this is you can call the feed tray or the composition of the pinch tray. So, similarly, I can write y, there is also this phase equilibrium j plus 1 is k i x i j plus 1 from the phase equilibrium.

So, if I combine this equation I mean combine the mass balance equation, combine the this intersection of the bottom and the stage and all this, as well as combine the equilibrium relation if I combine all of these equations I get this one.

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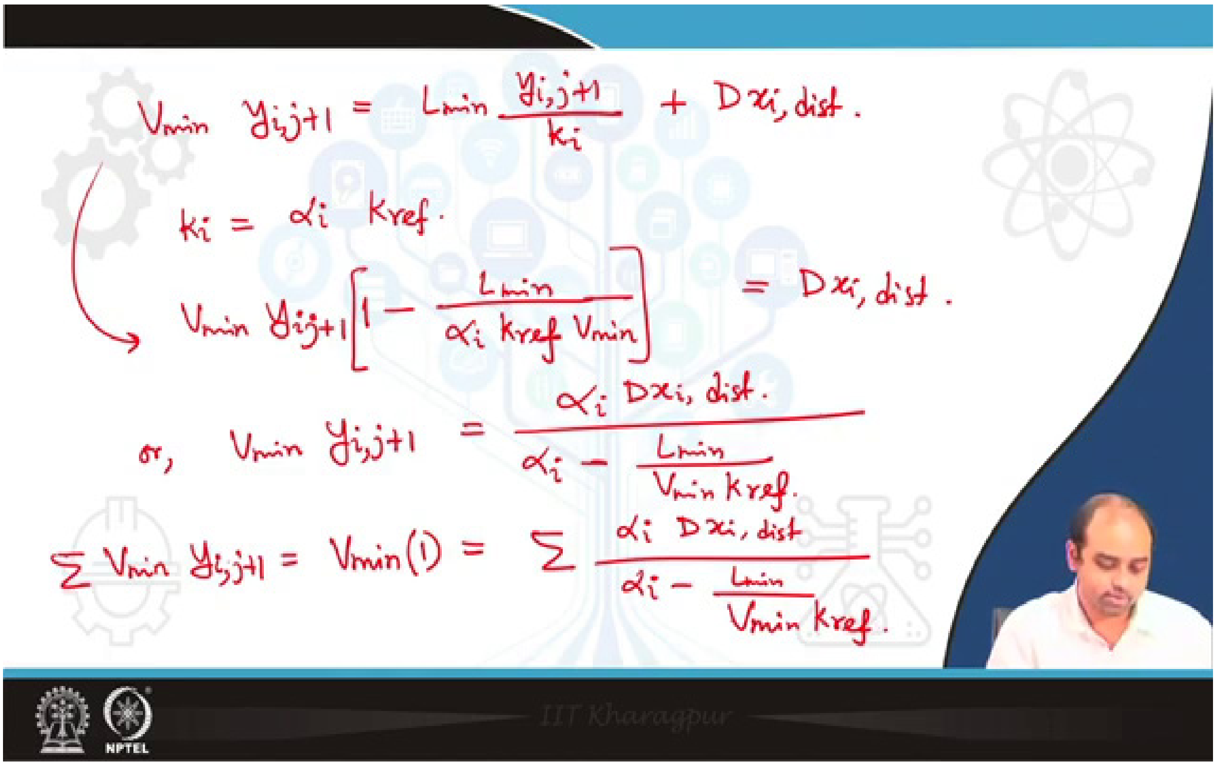

$$V_{min}\, y_{i,j+1} = L_{min} \frac{y_{i,j+1}}{k_i} + D x_{i,dist}.$$

$$k_i = \alpha_i\, K_{ref}.$$

$$V_{min}\, y_{i,j+1}\left[1 - \frac{L_{min}}{\alpha_i\, k_{ref}\, V_{min}}\right] = D x_{i,dist}.$$

$$\text{or,}\quad V_{min}\, y_{i,j+1} = \frac{\alpha_i\, D x_{i,dist}.}{\alpha_i - \frac{L_{min}}{V_{min}\, k_{ref}}}$$

$$\sum V_{min}\, y_{i,j+1} = V_{min}(1) = \sum \frac{\alpha_i\, D x_{i,dist}}{\alpha_i - \frac{L_{min}}{V_{min}\, k_{ref}}}.$$

Now, let us say for multi component specie with respect to a reference constant I can always write down that k i is equal to alpha i with respect to a reference value, this is always possible with respect to a reference component I can write down the relative volatility alpha in and to find out the equilibrium constant k I, this is always possible.

So, doing this gives me from this equation that I have V minimum y i j plus 1 minus L minimum divided by alpha i k ref, this is something I can write down is equal to D x i distillation. And from here I can write down as 1 minus of this quantity, this is something I can just write down so this is possible to get from here.

Of course, I have to write down as V minimum also here if I try to put the bracket, this is possible to write from this equation and subsequently I can also write this V minimum as y i j plus 1 is equal to D divide that I can also write multiply top and bottom with alpha i, so it is alpha i minus L min by V min k ref so these are all algebraic steps and I hope all of you are following and that is why I am doing little bit quickly.

Now, summation of V min y i j plus 1 will give you V min because summation of all the vapor phase components will lead to 1 and this will be equal to the summation of alpha i D x i the distillation divided by alpha i minus L min by V min k ref so this is the summation.

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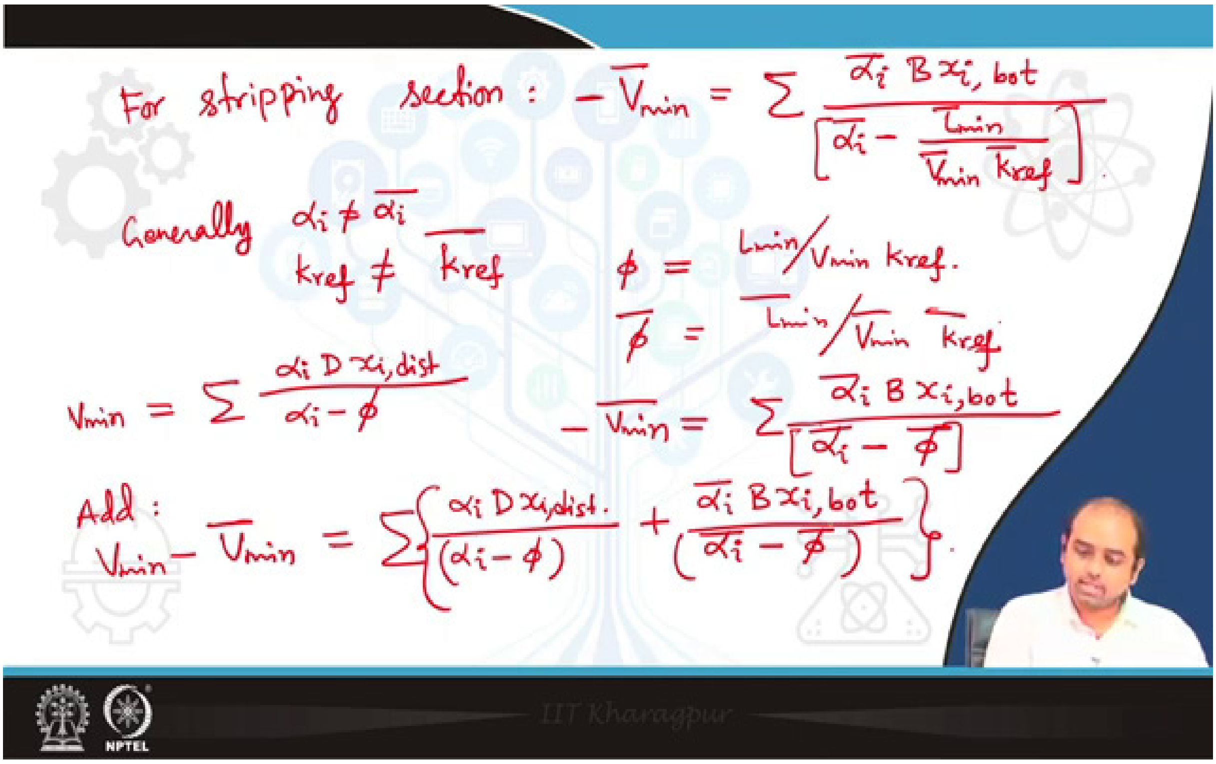

For stripping section : $-\bar{V}_{min} = \sum \frac{\bar{\alpha}_i B x_{i,bot}}{\left[\bar{\alpha}_i - \frac{\bar{L}_{min}}{\bar{V}_{min} \bar{k}_{ref}}\right]}$.

Generally $\alpha_i \neq \bar{\alpha}_i$

$k_{ref} \neq \bar{k}_{ref}$

$\phi = L_{min}/V_{min} k_{ref}$.

$\bar{\phi} = \bar{L}_{min}/\bar{V}_{min} \bar{k}_{ref}$

$$V_{min} = \sum \frac{\alpha_i D x_{i,dist}}{\alpha_i - \phi}$$

$$-\bar{V}_{min} = \sum \frac{\bar{\alpha}_i B x_{i,bot}}{[\bar{\alpha}_i - \bar{\phi}]}$$

Add :

$$V_{min} - \bar{V}_{min} = \sum \left\{ \frac{\alpha_i D x_{i,dist.}}{(\alpha_i - \phi)} + \frac{\bar{\alpha}_i B x_{i,bot}}{(\bar{\alpha}_i - \bar{\phi})} \right\}.$$

So, for stripping section same equation can also be obtained, I am not doing that calculation here but for stripping section you can also get the same equations, let us write that as using bar just to segregate the stripping and then reaching section, instead of distillate you will get at the bottom.

So, generally this alpha i is not equal to the alpha i bar as well as k ref in the stripping and the enriching section is not equal. So, let us define two quantities phi as something like L minimum by V minimum k ref, similarly, phi bar is equal to L minimum so this is like this ratio fractions in the stripping and the enriching section.

So, from here I mean if I combine this phi and if I reproduce this phi what I get is this V minimum for the enriching section I have alpha i D x i at the top divided by alpha i minus phi, so this is for the enriching section I have and from the stripping section I have V min bar

I mean minus of V min bar as summation of alpha i bar B x i at the bottom divided by this is something we have at the top.

Now, if you add these two V mins what you get? So, V min minus V min bar is equal to the summation of these two quantities, alpha i D x i distillate divided by alpha i minus phi plus alpha i bar B x i bottom as alpha i bar minus phi bar.

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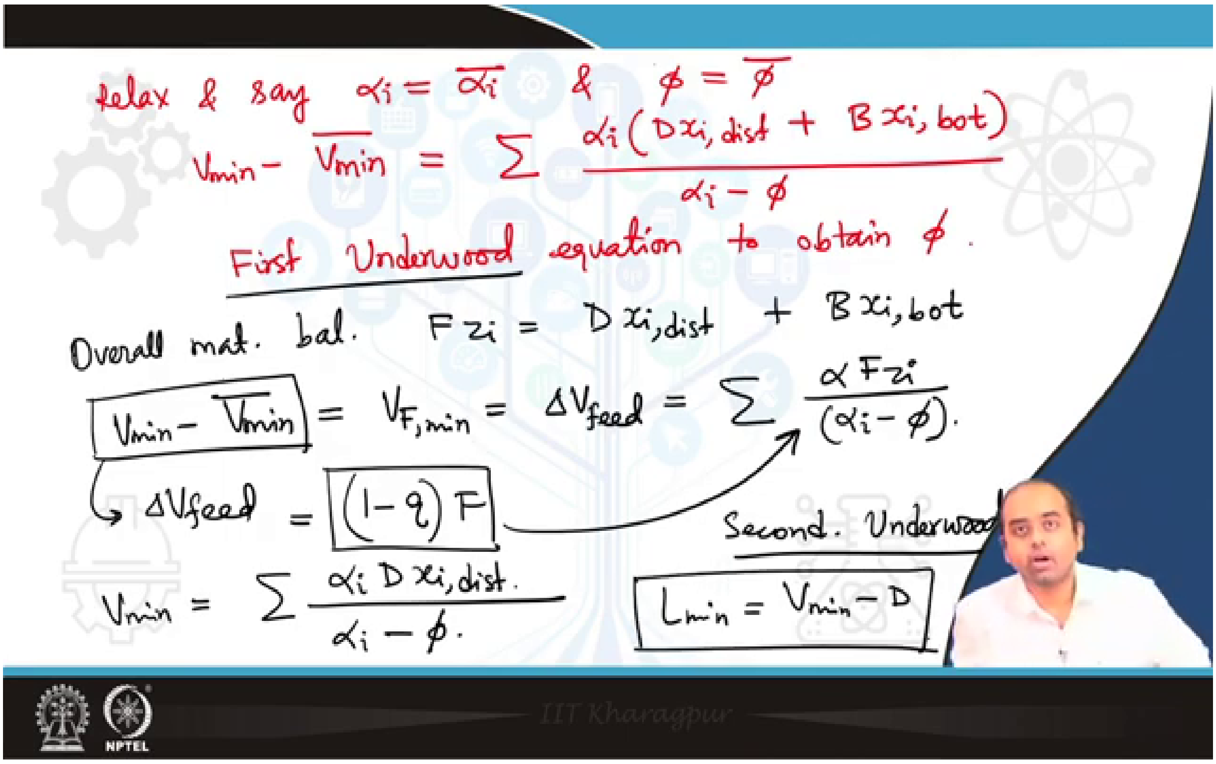

Relax & say $\alpha_i = \bar{\alpha_i}$ & $\phi = \bar{\phi}$

$$V_{min} - \bar{V_{min}} = \sum \frac{\alpha_i (D x_{i,dist} + B x_{i,bot})}{\alpha_i - \phi}$$

First Underwood equation to obtain ϕ.

Overall mat. bal. $F z_i = D x_{i,dist} + B x_{i,bot}$

$$\boxed{V_{min} - \bar{V_{min}}} = V_{F,min} = \Delta V_{feed} = \sum \frac{\alpha F z_i}{(\alpha_i - \phi)}.$$

$$\Delta V_{feed} = \boxed{(1-q)F}$$

Second Underwood

$$V_{min} = \sum \frac{\alpha_i D x_{i,dist}}{\alpha_i - \phi}.$$

$$\boxed{L_{min} = V_{min} - D}$$

So, now if you relax this idea that alpha is not equal to alpha i so if you relax this criterion and say that look that we are going to consider a sort of uniform alpha for the entire domain. So, if you relax the criteria and say that alpha i in the enriching section is same as the alpha i in the stripping section and this phi in the stripping and the enriching section are same then we get V min minus V min bar is equal to summation of alpha i D x i, distillation plus the top B x i, bottom divided by alpha i minus phi this is something we can do.

So, this is the first Underwood equation to obtain phi. And generally, how do you obtain this V min minus V min bar is using the material balance. So, let us say from overall material balance we know that F Z i is equal to D x i at the top plus B, this is something we know. So, we can write V min minus V min bar is equal to let us say V F. And what is this delta V?

So, difference of the vapor flow rates in the enriching and in the stripping section is equal to the amount of vapor present in the feed. So, delta V in the feed divide by the F is nothing but 1 minus q all of you are aware of what do you mean by q, q is the ratio of the amount of this liquid component in the feed, so 1 minus q is V, so delta V feed is equal to 1 minus q into F.

So, that is how you will get this difference. So, delta V is nothing but the difference of this quantity. So, from here you can relate back and you can find out, F is known, q is known, so from this equation essentially this relating this equation this one with this one will help you to find out what is your phi and once you find out what is your phi, so from the previous case, this is essentially the second Underwood equation, so the second Underwood equation.

So, this is the first Underwood equation, this is the second Underwood equation and then once you are able to calculate your phi, you know already this relation that V min is this quantity divided by alpha i minus phi. So, you already know what is your phi from this and then you can work out what would be your V minimum.

So, if your V minimum you can also calculate your L minimum which is V minimum minus D. So, in this way you can work out what would be your reflux ratio to the problem, reflux ratio is nothing but L by D, so you can, that is something you can work it out. So, using these two relations.

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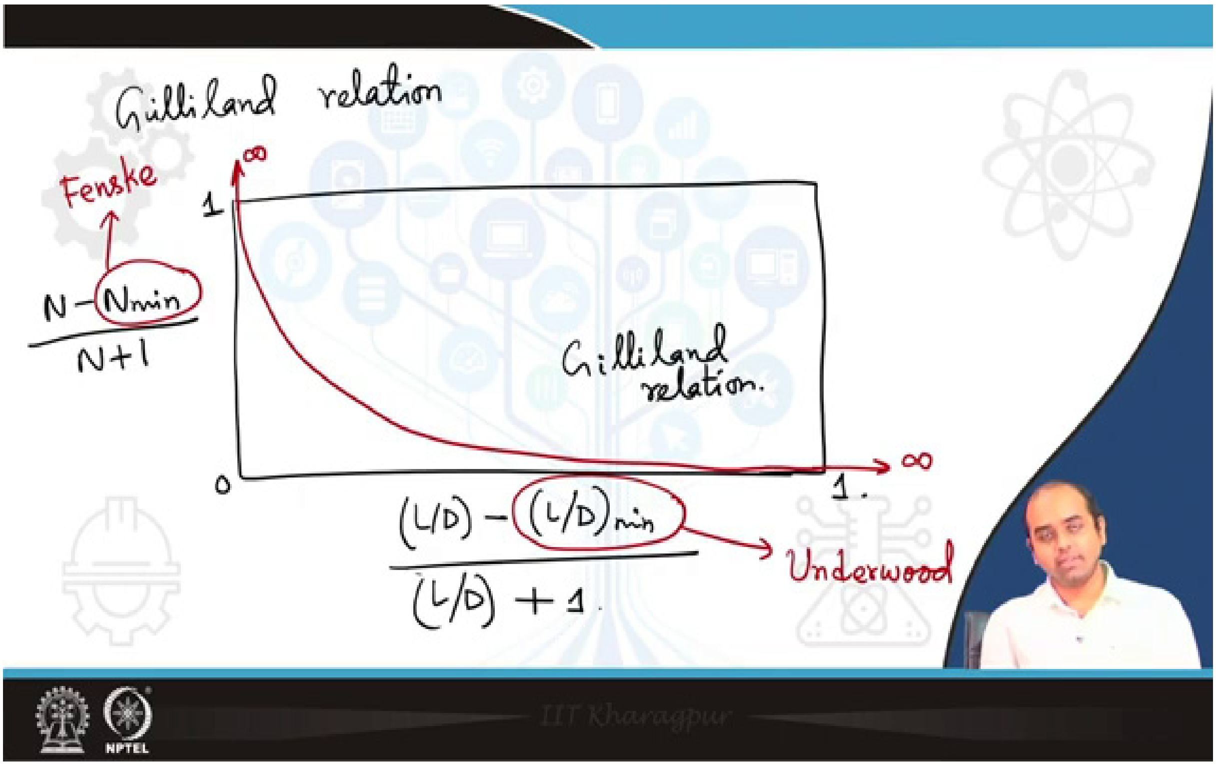

So, now that from the Fenske equation we can find out the number of stages for total reflux and from the Underwood equation we can calculate out what would be the minimum reflux ratio for infinite number of stages. So, the Gilliland equation is actually a chart though I am drawing it in a schematic but you can also find it anywhere in your, you just do a Google search this is something you will be able to find out.

So, on the left-hand side it is N minus N min divided by N plus 1 and at the bottom you have L by D minus L by D at the minimum condition divided by L by D plus 1, so this is starts from 0 to 1, so this is scaled with respect to 0 to 1 for this case. So, this is the Gilliland relation, this chart gives you see a relation of these quantities and of course you understood that from the N minimum is something to be obtained from the Fenske equation and L by D minimum has to be obtained from the Underwood equation at the criteria of minimum reflux or infinite stages and Fenske equation is for your total reflux.

So, if in your problem if the number of stages are specified then using this chart you can work out what would be the reflux ratio, if the reflux ratio is specified then you can work out what would be the number of stages and you see that these two cases correspond to the extreme cases. For example, if you are working with the case, if you are saying that you want minimum reflux ratio then the x coordinate becomes 0 and naturally the y coordinate turns out to be almost infinity that actually approaches to infinity, it is not actually to 1, it actually approaches to infinity in fact.

So, which tells you that the number of stages is infinity in that case. Again, in the case of number of this infinite, number of stages to be minimum if I select this number of stages to be minimum the curve reaches to a situation where it is almost tending towards infinity, so maybe I should draw a slightly better curve here to represent the infinity part, something like this, it does not actually touches the baseline or the y axis line. So, this also tends towards infinity, this also tends towards infinity.

So, I hope all of you have liked this class on, this is actually a shortcut method of calculating the number of stages or the reflux ratio whichever is not specified based on the idea of the Fenske and the Underwood relations and which is coupled together using this Gilliland correlation. Thank you for listening and your attention in this class.