Process Control and Instrumentation

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Lecture - 4
Mathematical Modeling (Contd.)

Today, we will continue our discussion on Mathematical Modeling and we will develop today the mathematical modeling of a distillation column.

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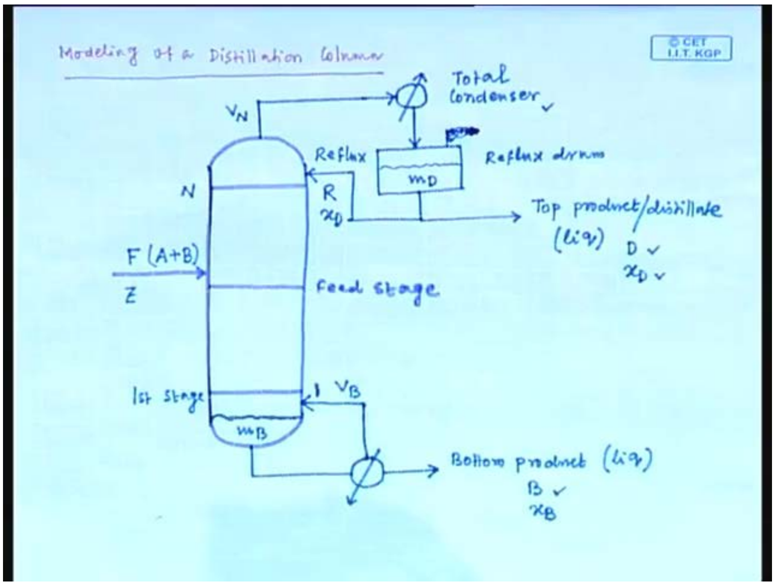

Modeling of a Distillation Column

Today, we will develop the model of a distillation column previously, we have configured three control scheme for a distillation column but, we did not discuss the modeling. So, first the configuration of a distillation column, this is the tower column section, this is the top tray, this is the feed tray and this is suppose, the bottom tray. Now, feed is introduced to this feed tray, this is the feed stage or feed tray, feed has the flow rate of F.

Suppose, this feed mixture contains only two components they are A and B, feed mixture contains two components namely A and B. The composition of this feed mixture is z now, the vapor which is living this top tray, this top tray is denoted by N. A vapor steam which is living this top tray has the flow rate of V N, the vapor steam which is living this top stage has the flow rate of V N. Now, this vapor steam is condensed in an over hit condenser, this is a condenser.

After condensation, the produced liquid, condensed liquid is accumulated in a drum, this is called reflux drum. The condensed liquid is accumulated in this reflux drum suppose, a holdup of this condensed liquid in the reflux drum is m D. If part of this accumulated liquid is withdrawn as top product, this is top product, this is also called distillate, top product is also called distillate and definitely, this is a liquid steam. Now, we will assume the flow rate of this distillate is D and composition is x suffix D.

The top product flow rate we are representing by capital D and composition is by x D, a fraction of this accumulated liquid is recycled back to the top tray, this stream is called reflux stream. This reflux stream has the flow rate of R and composition is same with the distillate steam I mean, the composition is x D. Similarly, at the bottom section, the liquid which left this bottom tray, this is we can say first tray, this is first stage, the liquid which is living this first stage is accumulated in this column base.

Suppose, the holdup in the column base is m suffix B now, this liquid then goes to a bottom reboiler and vaporization of liquid occurs in this reboiler. Then, the vaporized stream is recycle back to the bottom stage suppose, this vapor flow rate is V suffix B, the flow rate of this recycle vapor is suppose V B and the part of that accumulated liquid in the column base is withdrawn as bottom product. This is bottom product, this is also a liquid stream, it has the flow rate of suppose B and composition is x B, the flow rate of this bottom product is suppose B and composition is x B.

So, we are basically introducing to this column is single feed stream and we are getting two products, top product and bottom product. Now, this condenser is basically a total condenser, the operate condenser is actually a total condenser because, the operate vapor is totally condensed, the operate vapor which is entering the condenser is totally condensed. We can call this condenser as a partial condenser, there is a operate vapor distillate in forward.

When there is operate vapor distillate involve then, we can only say this is a partial condenser but here, we are considering, it is a total condenser so, there is no operate vapor withdrawn. So, this is all about the description of the distillation operation next, will develop the model based on some assumptions so, what are these assumptions.

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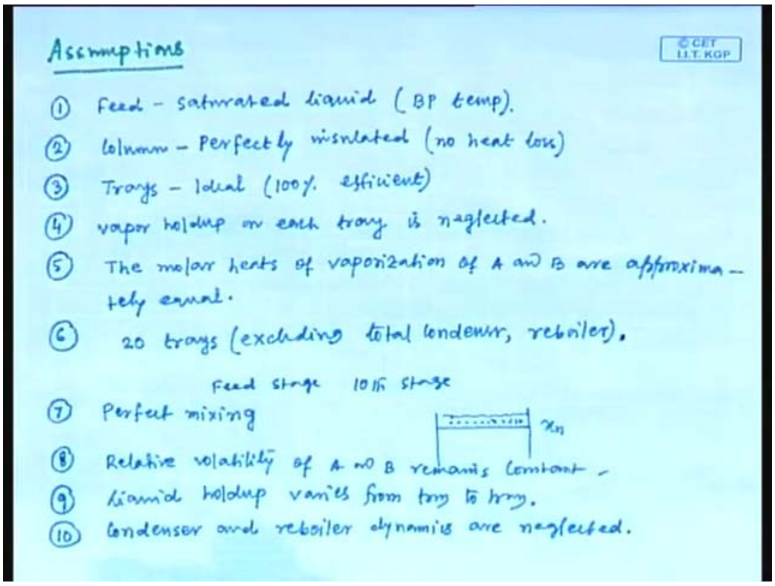

Assumptions

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① Feed - saturated liquid (BP temp).

② Column - Perfectly insulated (no heat loss)

③ Trays - Ideal (100% efficient)

④ vapor holdup on each tray is neglected.

⑤ The molar heats of vaporization of A and B are approximately equal.

⑥ 20 trays (excluding total condenser, reboiler).

Feed stage 10th stage

⑦ Perfect mixing

⑧ Relative volatility of A and B remains constant.

⑨ Liquid holdup varies from tray to tray.

⑩ Condenser and reboiler dynamics are neglected.

First assumption is, feed is a saturated liquid, the feed which is entering into the column that is a saturated liquid that means, the feed is at it is boiling point temperature, this is the first assumption. Second assumption is, the column is perfectly insulated that means, there is no heat loss from the distillation column to the surroundings. It means, no heat loss from the process to the surroundings, the column is insulated so that, there is no heat loss from the column to the surroundings.

Third assumption is, all the trays are ideal that means, the trays are 100 percent efficient or we can say, tray efficiency is 100 percent so, in this column, we are considering ideal trays, 100 percent efficient trays. Next assumption is, there is no vapor holdup, vapor holdup on each tray is neglected because, the density of vapor is much, much lower than the density of liquid that is why, we are considering this. For the high presser column, this assumption is taken into account I mean, the vapor holdup is considered on each tray.

Fifth assumption is, the molar heats of vaporization of both components A and B are approximately equal. It implies that, 1 mole of condensing vapor releases sufficient heat to vaporize 1 mole of liquid that means, for the condensation of the vapor, some heat is evolved. I mean, the vapor which is condensed, that releases some amount of heat and for vaporization of liquid, heat is required. Now, the 1 mole of condensing vapor releases the heat that is sufficient to vaporize exactly 1 mole of liquid, the meaning of this assumption is that.

Sixth assumption is, the column has total 20 trays excluding total condenser and reboiler, although this is not the assumption, this is basically the configuration of the process but anyway, we have included under assumptions. So, we have considered N for to represent the top stage basically, N is 20 here, seventh one is anyway, we can include another thing with this, the feed stage is the tenth stage. So, feed stage is the tenth stage, the feed enters the column on ten stage, seventh assumption is perfect mixing on each stage.

That means, if this is a tray suppose, this is the liquid stream so, if we consider perfect mixing on each tray then, composition of the liquid everywhere same I mean, if we represent the composition x N, that is identical everywhere on this stage. Next assumption is, relative volatility of the two components A and B remains constant throughout the column.

Next assumption is nineth assumption, liquid holdup varies from tray to tray, our fourth assumption is negligible vapor holdup but, we are considering liquid holdup I mean, liquid holdup varies from tray to tray but, there is no variation of vapor holdup. Last assumption tenth that is, condenser and reboiler dynamics are neglected, we are not considering the dynamics of condenser and reboiler. So, based on this ten assumptions, we will develop the model for the binary distillation column now, you just see, you just visit the assumptions 2, 4 and 5.

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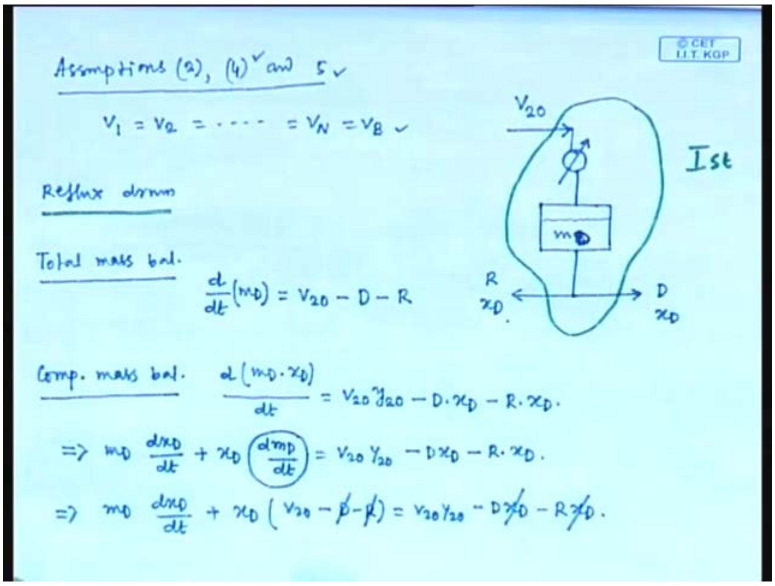

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Assumptions (2), (4) ✓ and 5 ✓

$V_1 = V_2 = \cdots = V_N = V_B$ ✓

Reflux drum

Total mass bal.

$$\frac{d}{dt}(m_D) = V_{20} - D - R$$

Comp. mass bal.

$$\frac{d(m_D \cdot x_D)}{dt} = V_{20} y_{20} - D \cdot x_D - R \cdot x_D.$$

$$\Rightarrow m_D \frac{dx_D}{dt} + x_D \boxed{\frac{dm_D}{dt}} = V_{20} y_{20} - D x_D - R \cdot x_D.$$

$$\Rightarrow m_D \frac{dx_D}{dt} + x_D (V_{20} - \cancel{D} - \cancel{R}) = V_{20} y_{20} - \cancel{D x_D} - \cancel{R x_D}.$$

Revisit assumptions 2, 4 and 5, second assumption is, the column is perfectly insulated that means, there is no heat loss. Now, this fourth assumption is, there is no vapor holdup, vapor holdup is negligible on each tray and fifth assumption is, if 1 mole of vapor condenses, at the same time 1 mole of liquid is evaporated. Can we write based on this three assumptions, all the vapor flow rates are identical I mean, the vapor stream which is living first tray equals to the vapor living second stage like this way, the vapor living N stage equals to V B, can we write.

So, based on the assumptions 2, 4 and 5, we can write that all the vapor flow rates throughout the column, they are identical it means, V 1 equal to V 2 equal to V N finally, V B. Anyway next, we will go to develop the modeling equations dividing the distillation column into different envelope. So, first we will develop the modeling equation for the top section, top section means, reflux drum. So, first we will develop the modeling equation for reflux drum, the schematic of a reflux drum is like this, this is the reflux drum.

Since we have considered there is no dynamics of condenser so, we can include here without developing any modeling equation for the condenser. The vapor stream which is entering into the condenser that we have represented previously by V N, N is basically 20 because, we have consider total number of stages 20. Now, this is the accumulation of liquid in the reflux drum suppose, the liquid holdup is m D, there are two outgoing streams, one is distillate composition is x D, another one is R composition is x D.

See, all the compositions are here basically the mole fraction, you consider all the compositions as mole fractions and flow rates are here basically molar flow rate say, for the example, D has the unit of mole per unit time. Now, this is the schematic of the top section and we will consider this as the first envelope, this is the first envelopes. Now, we have to develop basically the two equations, one is total mole balance and another one is component mole balance.

So, what will be the total, we will write here total mass balance originally, that is mole balance and we will writing here, total mass balance. Now, differentiation of m D, this is accumulation, what is the input to this envelope, V 20. V 20 is the input to this envelopes, what are the outputs, one is D and second one is R so, d m D d t equals to V 20 minus D minus R, this is a total mass balance equation for this first envelope.

Next, we will develop the component mass balance equation, what will be the component mass balance equation d m D multiplied by x D d t, equals to V 20 what is the composition, this is vapor steam. So, vapor composition will represent by y and liquid composition will represent by x so, V 20 multiplied by y 20, agree vapor flow rate is V 20 and it is composition is y 20. Now, D multiplied by composition, what is the composition of distillate x D similarly, R multiplied by x D, the composition of reflux stream is x D.

So, this is the component mole balance equation or component mass balance equation now, you use to simply this equation. So, m D d x D d t plus x D d m D d t equals to V 20 y 20 minus d x D minus R x D, we will substitute here d m D d t tomb. So, m D d x D d t plus x D, what is d m D d t that is, V 20 minus D minus R equal to V 20 y 20 minus D x D minus R x D. So, this D x D, this D x D will be canceled similarly this and this, R x D and R x D so, what will be the final expression.

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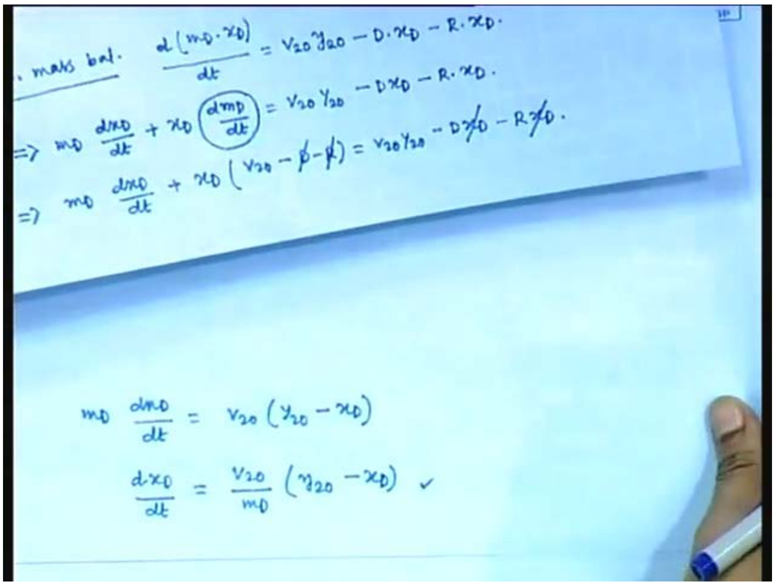

. mass bal.

$$\frac{d(m_D \cdot x_D)}{dt} = V_{20} y_{20} - D \cdot x_D - R \cdot x_D.$$

$$\Rightarrow m_D \frac{dx_D}{dt} + x_D \boxed{\frac{dm_D}{dt}} = V_{20} y_{20} - D x_D - R \cdot x_D.$$

$$\Rightarrow m_D \frac{dx_D}{dt} + x_D \left(V_{20} - \cancel{D} - \cancel{R}\right) = V_{20} y_{20} - D\cancel{x_D} - R\cancel{x_D}.$$

$$\Rightarrow m_D \frac{dx_D}{dt}$$

$$m_D \frac{dx_D}{dt} = V_{20} (y_{20} - x_D)$$

$$\frac{dx_D}{dt} = \frac{V_{20}}{m_D} (y_{20} - x_D) \checkmark$$

Final expression will be m D d x D d t equals to V 20 y 20 minus x D, if we further simplify we will get, D x D d t equal to V 20 by m D y 20 minus x D. So, this is the final form of component mass balance equation for first envelope, envelope 1 now, in the next, we will consider the second envelope that is, the top stage.

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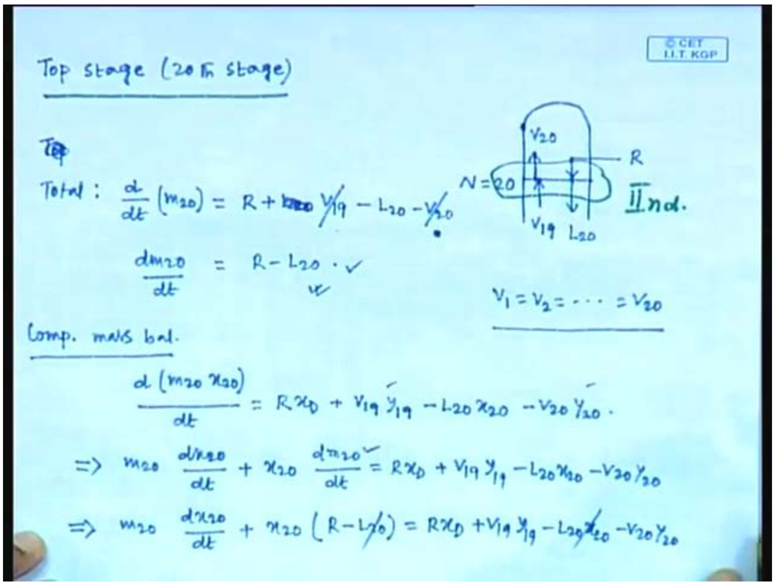

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Top stage (20th stage)

Top

Total: $\frac{d}{dt}(m_{20}) = R + \cancel{V_{19}} - L_{20} - \cancel{V_{20}}$

$$\frac{dm_{20}}{dt} = R - L_{20}. \checkmark$$

$V_1 = V_2 = \cdots = V_{20}$

Comp. mass bal.

$$\frac{d(m_{20} x_{20})}{dt} = R x_D + V_{19} y_{19} - L_{20} x_{20} - V_{20} y_{20}.$$

$$\Rightarrow m_{20} \frac{dx_{20}}{dt} + x_{20} \frac{dm_{20}}{dt} = R x_D + V_{19} y_{19} - L_{20} x_{20} - V_{20} y_{20}$$

$$\Rightarrow m_{20} \frac{dx_{20}}{dt} + x_{20} \left(R - \cancel{L_{20}}\right) = R x_D + V_{19} y_{19} - L_{20}\cancel{x_{20}} - V_{20} y_{20}$$

So, next we will consider the top stage, that is twentieth stage, first we have to make the schematic for this so, this is the top section of the column and this is twentieth stage so, N equals to 20. Now, the vapor which is living this top stage that is, V 20 what is the incoming to this stage, one is reflux R and another one is the vapor steam, which is coming from nineteen stage that means, V 19. Outgoing steams one already we have drawn, that is V 20, another one will be L 20.

So, incoming sterams are, one is V 19, another one is R, outgoing streams are L 20 and V 20 so, this is the second envelope. Similarly, we have to develop the total mass balance equation, we will consider for this twentieth stage, the liquid holdup as N 20. If the liquid holdup is m 20 then, d d t m 20 which is basically the accumulation term, equals the input flow rates. What are the input flow rates, one is R, another one is V 19 and outgoing streams are L 20 minus V 20, input minus output.

Now, based on the second, fourth and fifth assumptions we have concluded that, all the vapor flow rates are identical. If that is the case so, V 19, V 20 they are identical so, V 19 and V 20 they are equal to each other. Now, this equation reduces to R minus L 20, got it since based on the assumptions 2, 4 and 5 we have concluded that, all this vapor flow rates are same, if that is the case, we have to cancel out this V 19 and V 20. Then finally, we get the total mass balance equation d m 20 d t equals to R minus L 20.

What will be the component mass balance equation, component mass balance d m 20 corresponding composition is, x 20 d t equal to reflux flow rate and composition x D plus V 19 y 19 minus L 20 x 20 minus V 20 y 20. Why you did not multiply the composition with this equation final form I mean, why we have included again V 19 and V 20 terms in the component mass balance equation. Because, x is varying from tray to tray and y basically, is the equilibrium composition of x.

So, y varies to tray to tray that is why, we cannot neglect these two terms from this component mass balance equation. Can we simplify this equation, as we did for the case of first envelope so, m 20 d x 20 d t plus x 20 d m 20 d t equals to R x D plus V 19 y 19 minus L 20 x 20 minus V 20 y 20. If we substitute the total mass balance x 20 d t plus x 20 d m 20 d t, we will substitute that is, R minus L 20 equals to R x D plus V 19 y 19 minus L 20 x 20 minus V 20 y 20 so, L 20 x 20 is cancelled out.

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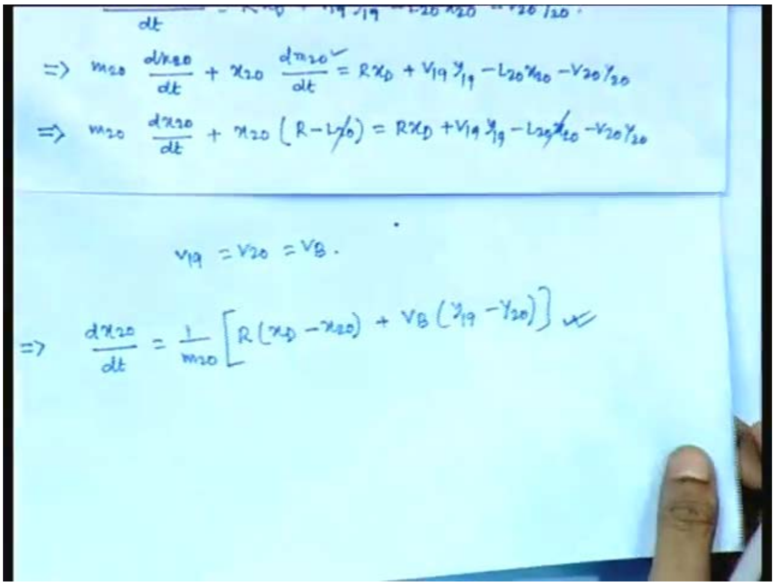

$$\Rightarrow m_{20}\frac{dx_{20}}{dt} + x_{20}\frac{dm_{20}}{dt} = Rx_D + V_{19}y_{19} - L_{20}x_{20} - V_{20}y_{20}$$

$$\Rightarrow m_{20}\frac{dx_{20}}{dt} + x_{20}(R - \cancel{L_{20}}) = Rx_D + V_{19}y_{19} - \cancel{L_{20}x_{20}} - V_{20}y_{20}$$

$$V_{19} = V_{20} = V_B.$$

$$\Rightarrow \frac{dx_{20}}{dt} = \frac{1}{m_{20}}\left[R(x_D - x_{20}) + V_B(y_{19} - y_{20})\right]$$

So, finally, we will get d x 20 d t equal to 1 by m 20 R x D minus x 20 plus V B y 19 minus y 20, this is a component mass balance equation. Just we have substitute it, V 19 equals to V 20 equals to V B then, we get this equation. So, this is the second envelope, the modeling equations of the second envelope next, we will consider the third envelope.

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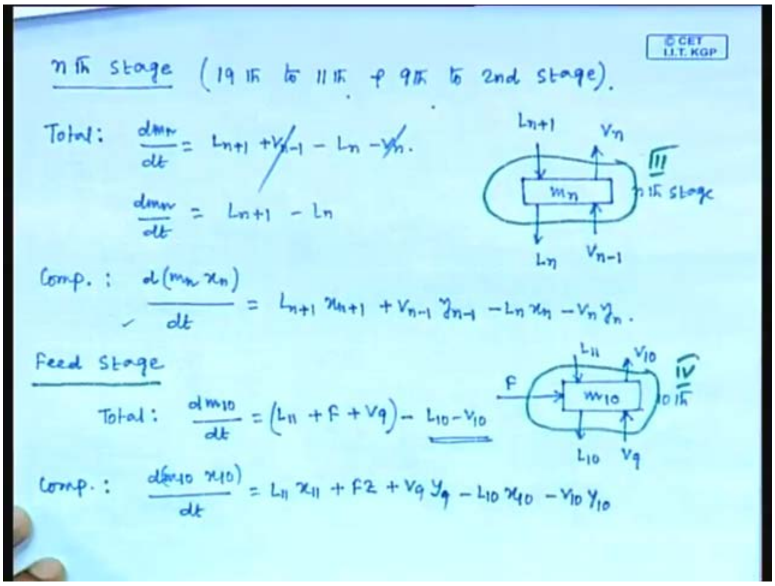

n th stage (19 th to 11 th & 9 th to 2nd stage).

Total: $\frac{dm_n}{dt} = L_{n+1} + \cancel{V_{n-1}} - L_n - \cancel{V_n}.$

$$\frac{dm_n}{dt} = L_{n+1} - L_n$$

Comp.: $\frac{d(m_n x_n)}{dt} = L_{n+1}x_{n+1} + V_{n-1}y_{n-1} - L_n x_n - V_n y_n.$

Feed stage

Total: $\frac{dm_{10}}{dt} = (L_{11} + F + V_9) - \underline{L_{10} - V_{10}}$

Comp.: $\frac{d(m_{10} x_{10})}{dt} = L_{11}x_{11} + Fz + V_9 y_9 - L_{10}x_{10} - V_{10}y_{10}$

That is any tray, will represent by any tray by n th tray so, n th stage now, this is the schematic of n th stage, holdup is m suffix n. Input streams are, one is V n minus 1 and another one is L n plus 1, outgoing streams are V n and another one is L n, this is a schematic of n stage. So, this is a third envelope, you quickly derive the modeling equations, what will be the total mass balance for this. D m n d t equals to incoming streams are L n plus 1 plus V n minus 1 and outgoing streams are L n minus V that means, the final expression is like this, d m n d t equals to l n plus 1 minus l n.

What will be the component mass balance, d m n x n d t equal to L n plus 1 x n plus 1 plus V n minus 1 y n minus 1 minus L n x n minus V n y n. It is quite strait forward to write the equation for component mass balance so, we will not proceed further to simplify this equation, it is quite easy. So, in the next any way so, what will be the n th stage basically, n th stage is basically just below the top stage that means, nineteenth to above the feed stages.

That means, eleventh stage and below the feed stage that means, nineth stage to above the bottom stage that means, second stage. Basically, we have considered common nomenclature n for this stages that is why, we have represented that by n stage and those are just nineteen to eleven and ninth to second stage. So, in the next, we will consider the feed stage, which is not included within this n stage, also the first stage is not included here.

Because, that has slightly different nomenclature similarly, for the case of column base, we have to consider to separately. So now, you will consider the feed stage, we will derive the total mass balance and component mass balance for the feed stage. So, first we have to draw the feed stage, this is the feed stage that is basically ten stage. So, the holdup will be m 10, one input stream that is feed stream, another one is L 11, the liquid which is coming from just above the feed tray. Another input is the vapor steam which is coming just below the feed tray that is, V 9 and outgoing steams are V 10 L 10.

So, this is the fourth envelope so, what will be the total mass balance equation, total mass balance equation will be d m 10 d t equals L 11 plus F plus V 9, these are input steams L 11, F and V 9. And what are the outgoing steams, one is L 10, another one is V 10, these two are the outgoing steam. So, it is straight forward to write the component mass balance equation, just multiplying the flow rates with their composition.

In the accumulation term, we have to multiply the holdup with composition so, d m 10 x 10 d t equals L 11 x 11 plus F, feed composition is z plus V 9 y 9 minus L 10 x 10 minus

V 10 y 10, this is a modeling equations for the feed stage. See, within the n th stage as I have mentioned, the bottom tray is not also included.

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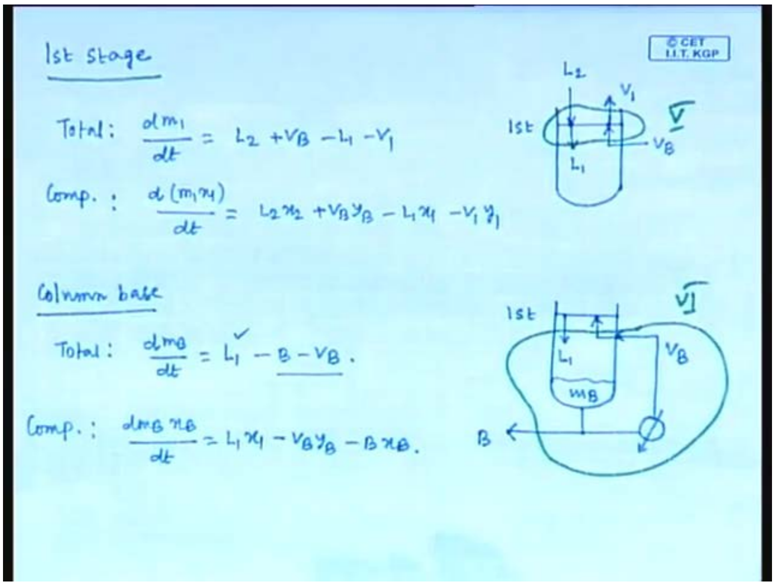

Ist stage

Total: $\frac{dm_1}{dt} = L_2 + V_B - L_1 - V_1$

Comp.: $\frac{d(m_1 x_1)}{dt} = L_2 x_2 + V_B y_B - L_1 x_1 - V_1 y_1$

Column base

Total: $\frac{dm_B}{dt} = \overset{\checkmark}{L_1} - \underline{B - V_B}$.

Comp.: $\frac{dm_B x_B}{dt} = L_1 x_1 - V_B y_B - B x_B$.

So, we will consider in the next the first stage, the schematic representation of the first stage is like this, this is the first stage. Now, input liquid flow rate one is L 2, another input steam is V B, which is coming from the reboiler. Outgoing streams are one is L 1, another one is V 1 so, this is the fifth envelope. What will be the total mass balance, if holdup is m 1 for the first stage then, d m 1 d t equal to L 2 plus V B minus L 1 minus V 1.

Similarly, component mass balance d m 1 x 1 d t equal to L 2 x 2 plus V B y B minus L 1 x 1 minus V 1 y 1, this is the component mass balance equation. The last envelope we have to consider that is the, column base which is also not included within n stage. So, last one is column base, the schematic of that is somewhat like this, this is the first stage and this is a column base. Some amount of liquid is accumulated in the column base, we are considering the holdup is m D and one reboiler is installed here.

This is the boiled up vapor which has the flow rate of V B, sometimes the bottom flow rate is included in this B. The liquid steam which is living first stage, that has the flow rate of L 1 and this V B is actually introduced to the first stage. So, what will be the total mass balance d m B d t equal to L 1, any way this is the sixth envelope so, total mass balance is d m B d t equals to input is L 1 and there are two output streams, one is B another is V B.

L 1 is a input stream, B and V B both are the outgoing steams from this sixth envelopes, what will be the component mass balance, d m B x B d t equal to L 1 x 1 minus V B y B minus V x B, this is the component mass balance equation. So basically, there are total six envelopes, one is for the reflux drum, second one is for top stage, third one is for n stage, fourth one is for feed stage, fifth one is for bottom stage and sixth one is for column base. Now, what are the variables involved in this modeling equations and how, we can calculate those variables.

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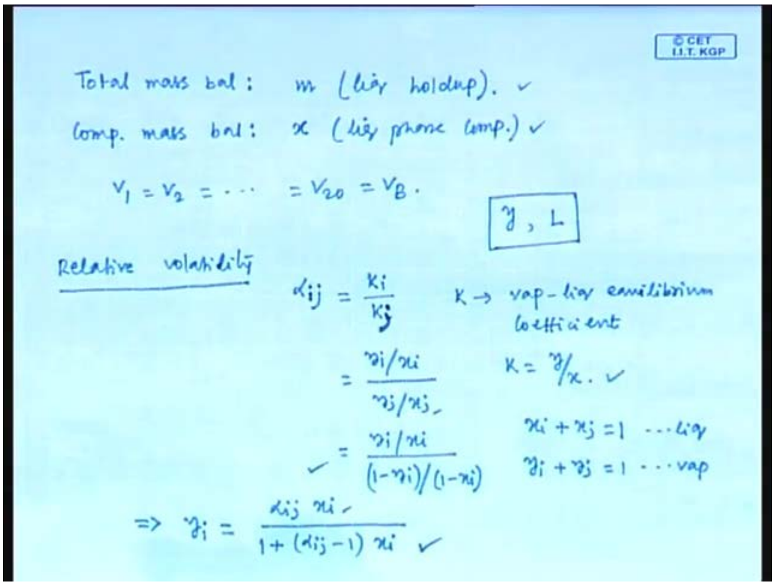

Total mass bal : m (liq holdup). ✓

Comp. mass bal : x (liq phase comp.) ✓

$V_1 = V_2 = \cdots = V_{20} = V_B$.

$\boxed{y, L}$

Relative volatility

$\alpha_{ij} = \frac{K_i}{K_j}$ K → vap-liq equilibrium coefficient

$= \frac{y_i/x_i}{y_j/x_j}$ $K = y/x$. ✓

$x_i + x_j = 1$ ...liq

$y_i + y_j = 1$ ...vap

✓ $= \frac{y_i/x_i}{(1-y_i)/(1-x_i)}$

$\Rightarrow y_i = \frac{\alpha_{ij} x_i}{1+(\alpha_{ij}-1)x_i}$ ✓

In the modeling equations, we got total mass balance, total mass balance equations are basically the ordinary deferential equations, by solving those equations what we can calculate, holdup. By solving the total mass balance equations which are basically the ordinary deferential equations, we can calculate holdup. Another type of modeling equations are based on component mass balance, this component mass balance equations are also ordinary differential equations.

By solving the component mass equation, we can get liquid phase composition and this is liquid holdup. So, m or total holdup liquid holdup and liquid phase composition, we can calculate from the developed modeling equations. Based on three assumptions second, fourth and fifth, we know all these vapor flow rates are identical, equal to V B.

So, this information is also known to us, all vapor flow rates we can calculate, what are the rest, one is y, another one is liquid flow rate.

How we can calculate these two variables, that we will discuss next, how we can calculate y. We assumed one thing that, the relative volatility of components A and B remains identical throughout the column, relative volatility is represented by alpha. So, relative volatility of any component i with respect to another component j is represented by alpha i j. Relative volatility is represented by alpha and the suffix is used in this way alpha i j means, relative volatility of component i with respect to component j. Alpha i j is related with k by this way I mean, alpha i j equals to k i divided by k j.

K is the vapor liquid equilibrium coefficient, it is also called distribution coefficient which is basically, represented by y by x I mean, k equals to y by x. So, can we write here, y i divided by x i whole divided by, this is for j not i, k i by k j. So, y i by x i whole divided by k j means, y j by x j, can we write this because, k equals to y by x so, we have just included here the suffix. Now, see our example column is a binary distillation column that means, there are two components, one is i and another one is j.

So, we can write x i plus x j equals to 1, this is for liquid phase similarly for vapor phase we can write, y i plus y j equals to 1, agree. Because, our mixture is a binary mixture now, we will write here, y i divided by x i whole divided by 1 minus y i divided by 1 minus x i. Our intension is to calculate, the vapor phase composition of component i that is why, we are trying to avoid y j and x j terms. So, y j equals to 1 minus y i and x j equals to 1 minus x I, if we rearrange this equation, we will get y i equals to alpha i j x i divided by 1 plus alpha i j minus 1 into x i.

If we rearrange this, finally we will get, y i equals to alpha i j x i divided by 1 plus alpha i j minus 1 into x i you see, in this equation, alpha i j is defined that is constant, we have assume that. X value we can calculate from the component mass balance equation so, all the terms in this equation are known except y i so, we can calculate y i. In the next class, we will discuss, how we can calculate the liquid flow rate L.