# Mathematical Modelling and Simulation of Chemical Engineering Process
**Professor Doctor Sourav Mondal**
**Department of Chemical Engineering**
**Indian Institute of Technology, Kharagpur**
## Lecture 39
## Multistage batch distillation

Hello everyone, In this class we are going to talk about this Multistage Batch Distillation process and of course, multistage as well as multicomponent batch distillation process taking the same inspiration from the mesh equations that we have talked about for the continuous distillation columns.

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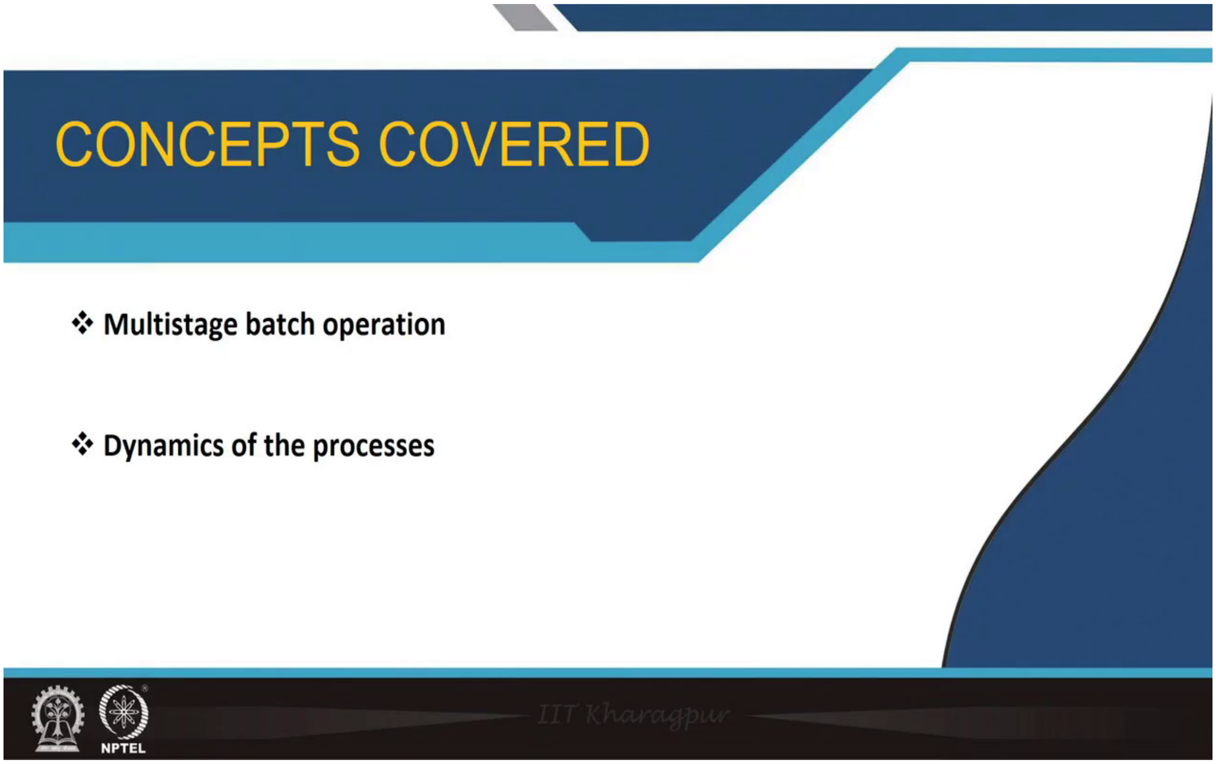

CONCEPTS COVERED

- Multistage batch operation
- Dynamics of the processes

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Now, so, here we are going to mostly talk about the idea of the dynamics of this process and you know that batch process are generally dynamical in nature and is a transient process. So, how we can frame the equations and how we can frame the, this structure of the equations as well as the calculation procedure for the batch process with the inspiration of the mesh equations from the continuous systems.

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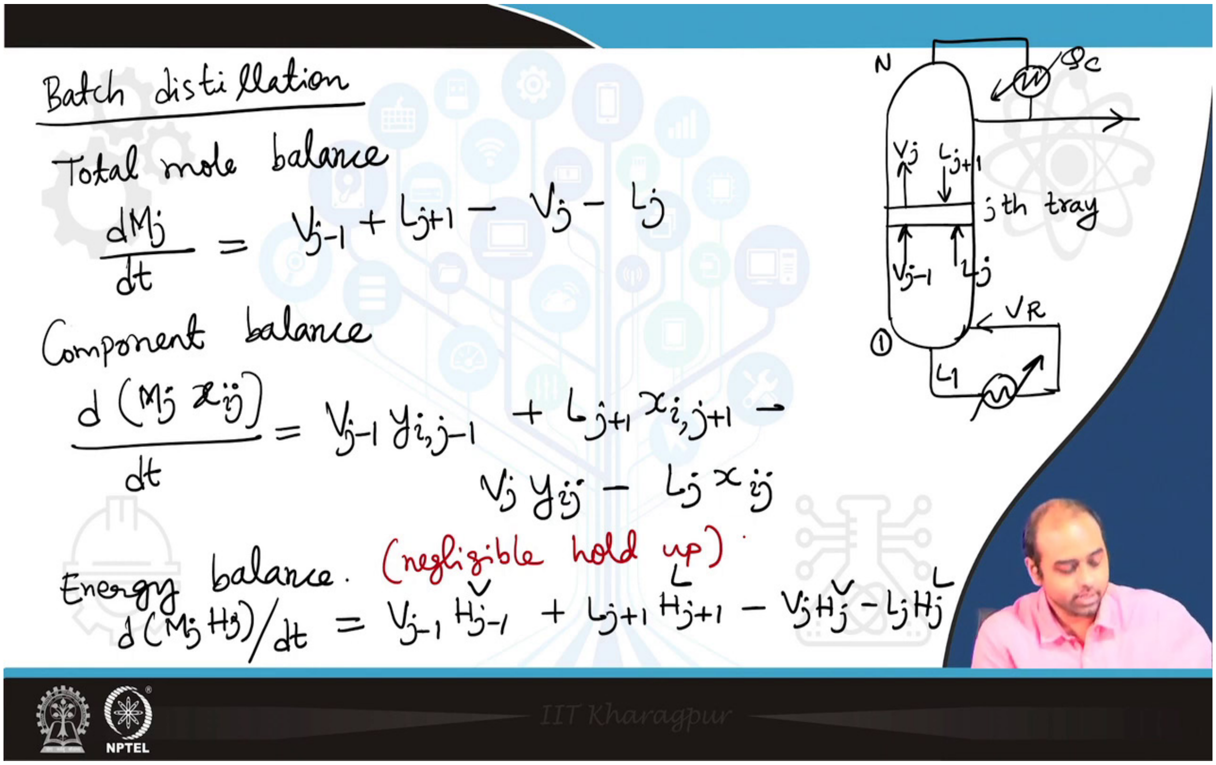

Batch distillation

Total mole balance

$$\frac{dM_j}{dt} = V_{j-1} + L_{j+1} - V_j - L_j$$

Component balance

$$\frac{d(M_j x_{ij})}{dt} = V_{j-1} y_{i,j-1} + L_{j+1} x_{i,j+1} - V_j y_{ij} - L_j x_{ij}$$

Energy balance. (negligible hold up)

$$d(M_j H_j)/dt = V_{j-1} \overset{V}{H}_{j-1} + L_{j+1} \overset{L}{H}_{j+1} - V_j \overset{V}{H}_j - L_j \overset{L}{H}_j$$

So, let us try to draw this simple distillation column here and mark this jth tray, so we follow the same pattern for j that the this is the jth tray. So, any stream that is leaving will take its you know indices so this is Lj plus, sorry j minus 1, so let us reverse the numbers here little bit, sorry, I take that as j plus 1 and this as j minus 1 this as Lj because I am considering the numbering from top to bottom, instead of bottom to top, just having a different way, is the reboiler.

So, whatever is getting from the reboiler market it as VR and you are having this condenser. And this is the heat load of the condenser market it as QC in this problem, so let us write the total so, it is a batch distillation system we are talking about. So, here the total mole balance we can write as in the jth tray as dMj this is the accumulation term or the transient term is Vj minus 1.

So, it is in minus out, so this is the in part and this is the out part component balance this is the component balance. So, we are having Vj minus 1, y is for the ith component plus L j plus 1 xij plus 1 and minus Vj yij minus of Lj xij, it is the component balance and the top we have written down the mole balance and the next one we have the energy balance, so d MjHj dt.

So, the left hand side is not equal to 0 now, there is a certain bit of transient or accumulation term exist. So, Vj minus 1 h j minus 1 I am writing that as for the vapor phase, then Lj plus 1. So, there is the enthalpy into the system H j plus 1 L that is the enthalpy out Vj Hj V and Lj Hj L. So, this is the enthalpy balance, of course, we are assuming that there is negligible holdup, so we are ignoring any hold up effects and all in this problem.

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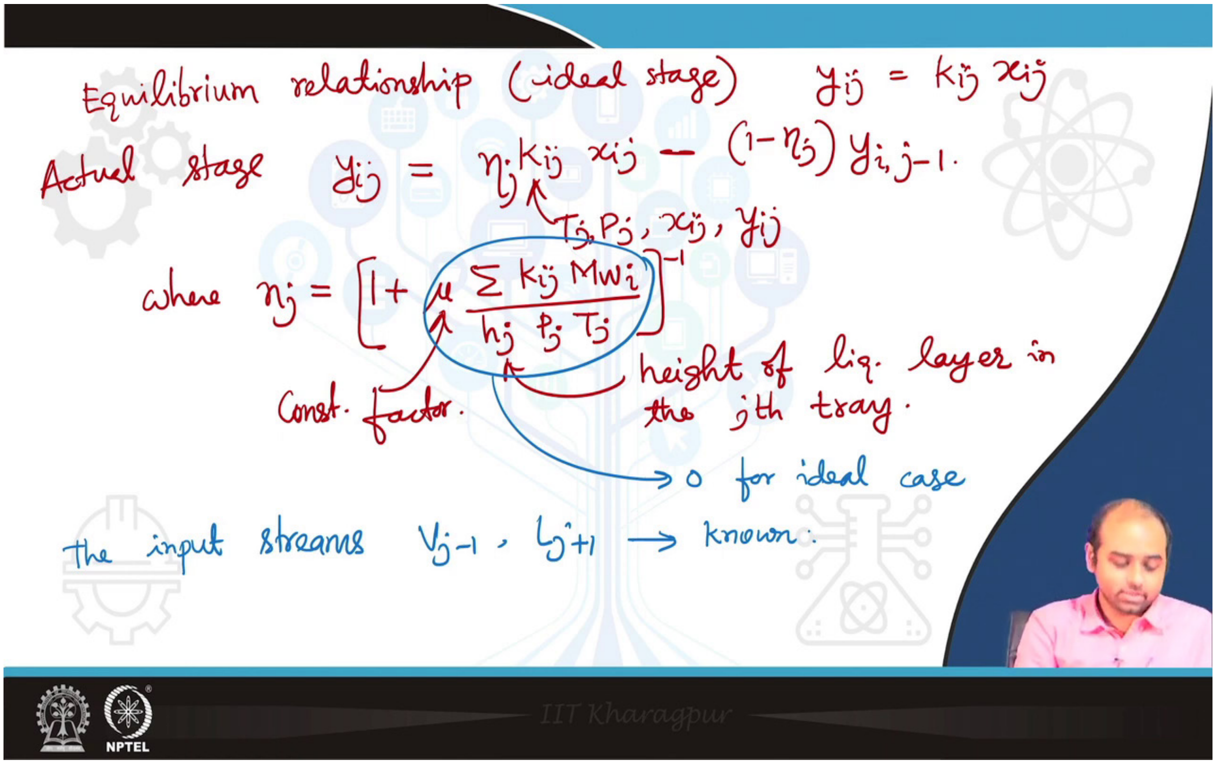

Equilibrium relationship (ideal stage) $y_{ij} = k_{ij} x_{ij}$

Actual stage $y_{ij} = \eta_j k_{ij} x_{ij} - (1-\eta_j) y_{i,j-1}$.

$T_j, P_j, x_{ij}, y_{ij}$

where $\eta_j = \left[1 + \mu \frac{\sum k_{ij} Mw_i}{h_j \rho_j T_j}\right]^{-1}$

Const. factor.

height of liq. layer in the jth tray.

→ 0 for ideal case

The input streams $V_{j-1}$, $L_{j+1}$ → known.

What about the equilibrium relationship? So, the ideal equilibrium relationship if we consider it to be ideal state then we can say that, yij is equal to kij xij but non ideal is the reality. So, the actual stage relationship yij will look can look something like, efficiency factor kij where this is a function of, of course Tj Pj.

And of course, different xij's and different yij's into xij minus 1 minus eta, sort of this free efficiency or plate efficiency you can consider where this efficiency factor eta j can is generally sometimes something is like a practical thing I am talking about this is not hj and let me write this as hj. So, this is actually from the tray hydraulics you can also get that, so this is height of liquid layer in jth tray and this mu is a constant factor.

So, in the ideal case, this entire factor goes to 0 for ideal case, you can think not ideal gas, ideal case you can think this mu to be equal to 0 or it is completely submerge the liquid layer is too high I mean if the liquid layer is also too high then you can expect this factor to be very low and the situation is more closer to the ideality.

So, all these tray hydraulics and the tray efficiencies you can look into the book by B. D. Smith on equilibrium stage equilibrium stage processes where very nicely it talks about distillation column design details about the tray hydraulics, the bubble cap columns and etc., and I am sure many of you may have already referred to it in your equipment design class. Now, what are the input streams?

So, the input streams in this formulation that is Vj minus 1 and Lj plus 1, these are known. So, the unknown is Lj and Vj. Now this Lj is something in this calculation we get it from the tray hydraulics.

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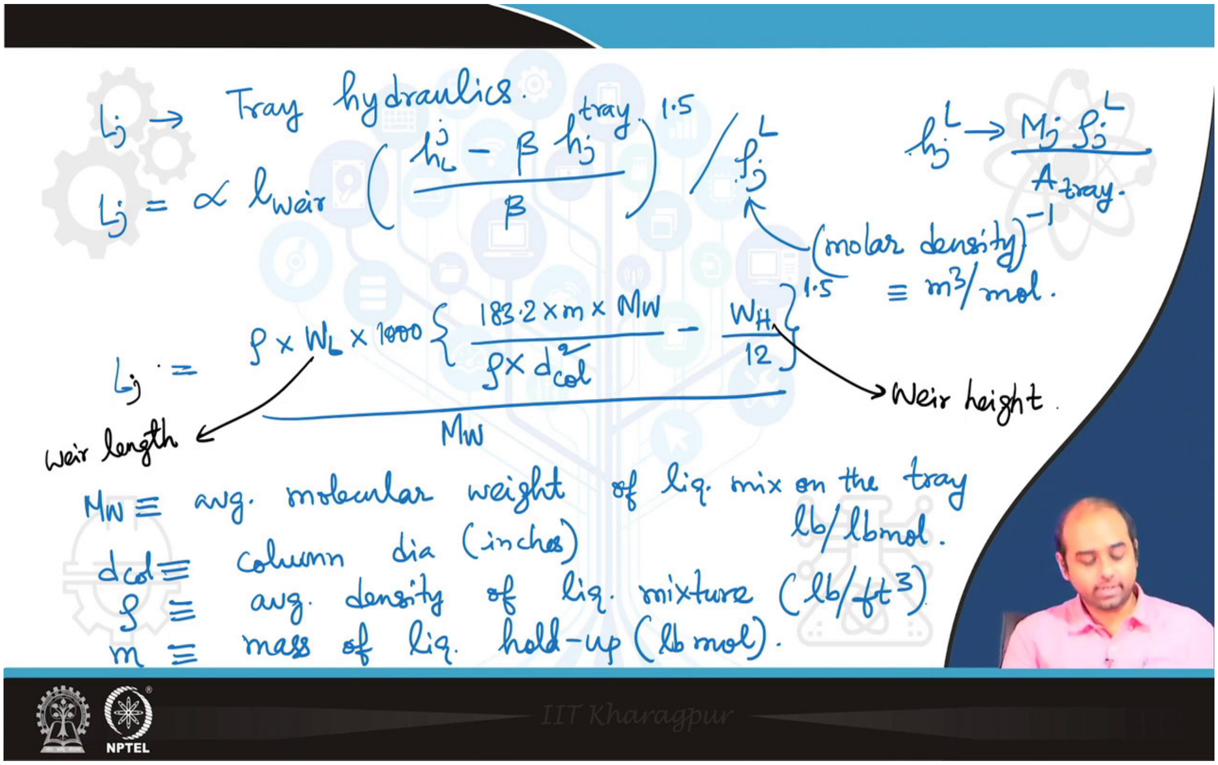

$L_j \rightarrow$ Tray hydraulics.

$$L_j = \alpha\, l_{weir} \left( \frac{h_L^j - \beta\, h_j^{tray}}{\beta} \right)^{1.5} \Big/ \rho_j^L$$

$$h_j^L \rightarrow \frac{M_j\, \rho_j^L}{A_{tray}}$$

$\rho_j^L \leftarrow$ (molar density)$^{-1}$ $\equiv m^3/mol$.

$$L_j = \frac{\rho \times W_L \times 1000 \left\{ \frac{183.2 \times m \times MW}{\rho \times d_{col}^2} - \frac{W_H}{12} \right\}^{1.5}}{MW}$$

weir length

Weir height.

$MW \equiv$ avg. molecular weight of liq. mix on the tray lb/lbmol.

$d_{col} \equiv$ column dia (inches)

$\rho \equiv$ avg. density of liq. mixture (lb/ft$^3$)

$m \equiv$ mass of liq. hold-up (lb mol).

So, Lj is actually obtained from the tray hydraulics. So, there are different versions of this formula you can have something like this based on the weir length and everything enthalpy values, there are several constants, this is one sort of the formula, the liquid holdup volume and here in this case this hj L is something M volumetric j by the area of the tray and this is nothing but better to write this is not volume but something like the rho in terms of let me write this in terms of density not in terms of volume.

So, this is the inverse of molar density, so this is something like metre cube per mole, so do not get confused as to be the densities so that is the reason why I wrote these things instead of density as like some sort of specific volume, so better to write so, this can be represented some sort of specific volume. So, volume per unit mole and there are different formulae, for example L can also be written down the liquid flow rate can also be written down in terms of this is another formula, let us say this as rho into WL into rho of some strange factors are there 1000.

Then it is multiplied with these numbers, so d column is the diameter of the column, square of that minus this Wh is the weir height 0.5 whole divided by the molecular weight. So, MW is the, this average molecular weight of the liquid mixture on the tray. So, this formula is based on pound mole per, sorry, lb pound per mole and that is why this strange you know numbers are there this d column is the is everything is in FPS unit column diameter in inches, then you have this rho which is the density of the liquid mixture.

So, this is given again in terms of pounds per feet cube all in FPS unit as I said, then you have this M, M is the mass of the liquid hold up in the tray in terms of pound mole and Wh and WL so this is weir length and this is weir height. So, generally there are also different types of other formulas you will find in different textbooks.

So, these are different formulas which have been the you know, formulated or proposed by different manufacturers at different point of time based on the column specifications or certain criteria in the column or from the operations. So, this is how do you get your liquid flow rate Lj in the column which is dependent mostly on the tray hydraulics.

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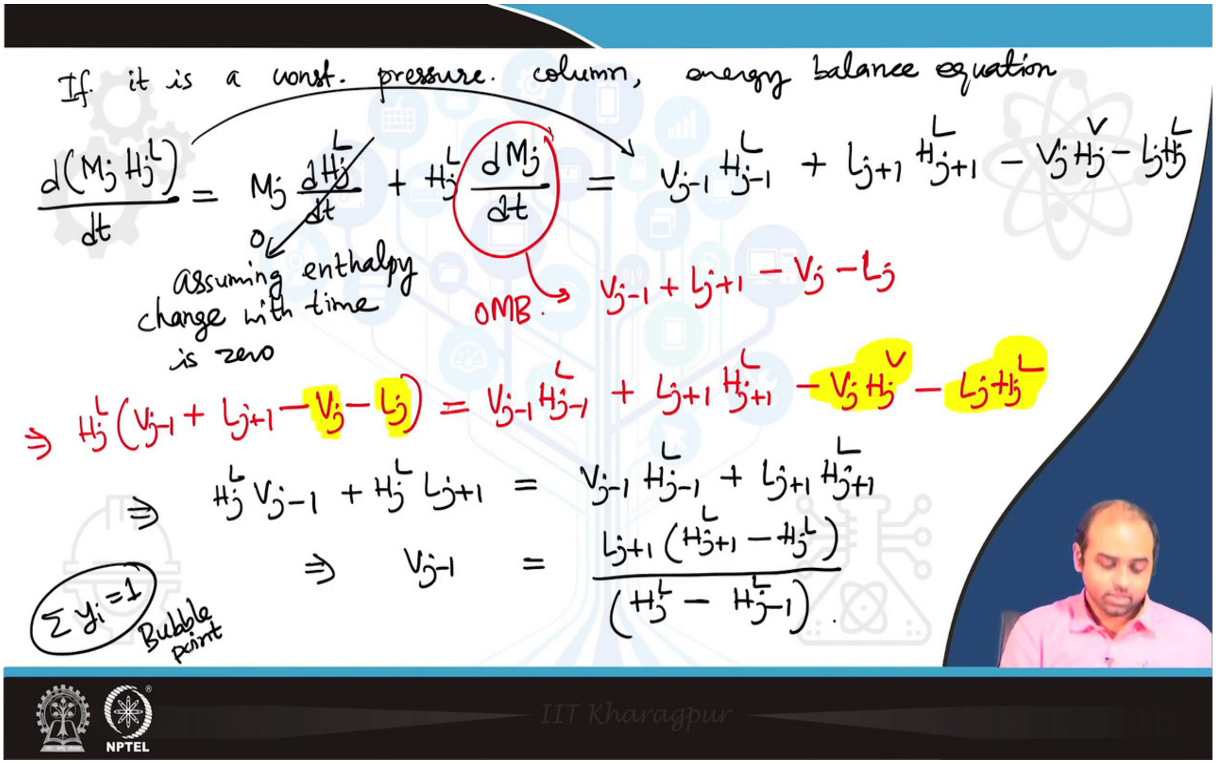

If it is a const. pressure column, energy balance equation

$$\frac{d(M_j H_j^L)}{dt} = M_j \underbrace{\cancel{\frac{dH_j^L}{dt}}}_{0} + H_j^L \boxed{\frac{dM_j}{dt}} = V_{j-1}H_{j-1}^L + L_{j+1}H_{j+1}^L - V_jH_j^V - L_jH_j^L$$

assuming enthalpy change with time is zero

$$\text{OMB} \rightarrow V_{j-1} + L_{j+1} - V_j - L_j$$

$$\Rightarrow H_j^L(V_{j-1} + L_{j+1} - V_j - L_j) = V_{j-1}H_{j-1}^L + L_{j+1}H_{j+1}^L - V_jH_j^V - L_jH_j^L$$

$$\Rightarrow H_j^L V_{j-1} + H_j^L L_{j+1} = V_{j-1}H_{j-1}^L + L_{j+1}H_{j+1}^L$$

$$\Rightarrow V_{j-1} = \frac{L_{j+1}(H_{j+1}^L - H_j^L)}{(H_j^L - H_{j-1}^L)}$$

$$\boxed{\Sigma y_i = 1}$$ Bubble point

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Now, what about the vapor flow rate? What about Vapor Vj in the system. So, if it is the constant pressure column, then you can consider the energy balance, the energy balance equation as d of Mj HjL dt as Mj dHjL dt and HjL dMj dt, let us say we consider this one as to be 0 assuming that the enthalpy change with time is 0 is setting that to be equal to 0. And of course, this on the right hand this is equal is already something we have written now Vj minus 1 Hj minus 1 L Lj plus 1 L Vj HjV Lj.

So, this quantity from the overall material balance we already know that this is equal to Vj minus 1 plus Lj plus 1 minus Vj minus Lj from mass balance, overall mass balance is something that you already know, now if you put in the numbers, some integers substitute everything here, so what do we get? This is the left hand side and the right hand side we already have. So now, if you match the left hand side and the right hand side, you can easily see that these quantities, these terms, these terms multiplied with Hj will be equivalent to these terms, isn't it?

And whatever this finally you are getting, equation in terms of your this sorry, I think I did a mistake here. You know it is fine. So, on the left hand side I am getting, no, it is fine. So, I am getting Hj L Vj minus 1 plus Hj L Lj plus 1 and this is equal to Vj minus 1 Hj minus 1 L plus Lj plus 1. So, from this equation I can get my Vj minus 1.

So, that is Lj plus 1 and I am getting Hj plus 1 L minus Hjl divided by Hj L minus H j minus 1 L. So, from here I can calculate out what is my Vj minus 1 and the last rho you already know that for the last rho that is VR that is something we can always calculate out from the reboiler conditions if I know my Lj and that will be equal to VR.

So, the last row it is VR then it will help you to calculate what is the last but previous rho provided you know all the specifications of the last rho. So, that is how you can work out and calculate your, this vapor phase calculations, sorry vapor flow rates. So, this Hj or this capital Hj the enthalpy is something that can be calculated from the tray temperatures, pressure and the liquid and the vapor compositions and provided you consider that the system is operating at the bubble point calculation.

So, at the bubble point at the bubble point this relation will always hold at bubble point. So, here you apply the this your equilibrium relationships and you can work out different temperatures, tray temperatures provided you can calculate out your Vj minus 1, I mean Vj so Vj from here you calculate and then the tray temperatures can be calculated based on the relation that this at the things are at the bubble point so you equate Yij, the tray composition or the vapor composition summation of the vapor tray composition is equal to 1.

Now, the question comes that if the pressure in the system is not constant then you have slightly different tricky situation. So, we can write something like this.

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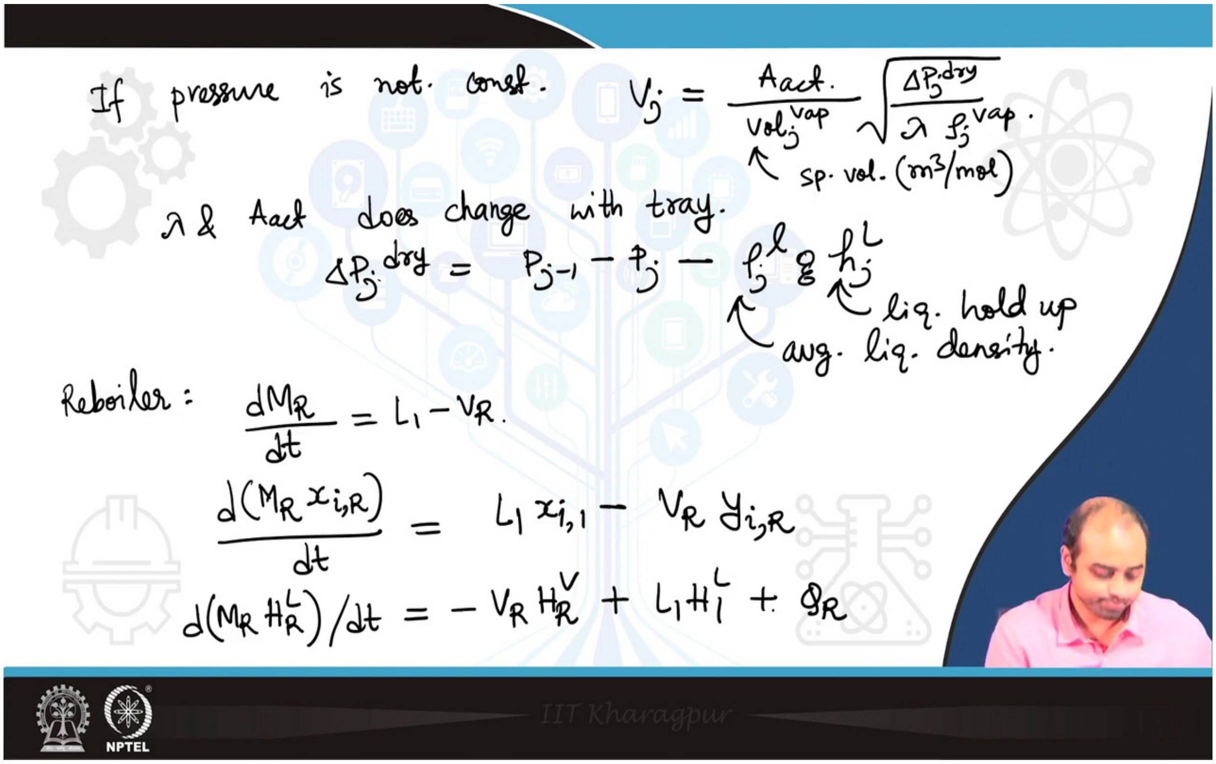

If pressure is not const. $V_j = \dfrac{A_{act.}}{Vol_j^{vap}} \sqrt{\dfrac{\Delta P_j^{dry}}{\lambda \rho_j^{vap}}}$.

↑ sp. vol. (m³/mol)

λ & Aact does change with tray.

$\Delta P_j^{dry} = P_{j-1} - P_j - \rho_j^{l} g h_j^{L}$

↑ liq. hold up

↑ avg. liq. density.

Reboiler: $\dfrac{dM_R}{dt} = L_1 - V_R$.

$$\frac{d(M_R x_{i,R})}{dt} = L_1 x_{i,1} - V_R y_{i,R}$$

$$d(M_R H_R^L)/dt = -V_R H_R^V + L_1 H_1^L + Q_R$$

So, if the pressure is not constant if pressure in the system is not constant, then the vapor flow rate Vj is given by this formula this is again the specific volume of the vapor. So, this is the specific volume in terms of meter cube per molar, inverse of density you can say square root of delta Pj dry lambda. So, this lambda and A are certain constants which depends on the tray.

So, this lambda and are does change with trays and this delta Pj dry is Pj minus 1 minus Pj minus any hydrostatic head that you may have due to the liquid hold up. So, this is the liquid holdup and this is the average liquid density in the tray. So, this is how you can calculate your Vj if pressure is not constant in the system and in that case, pressure becomes a variable using this relation you will relate your pressure and similarly then pressure is the unknown variable which needs to be quantified.

So now, let us look into the different balances of the different stages. So, for the case of the reboiler written down in terms of R dMR dt is nothing but L1 minus VR. Similarly, dMR dxi R all the difference, I mean for this is for the reboiler tray or the last stage comma 1 minus VR yi, R. Similarly, the enthalpy balance at the reboiler gives you this is the enthalpy balance at the reboiler.

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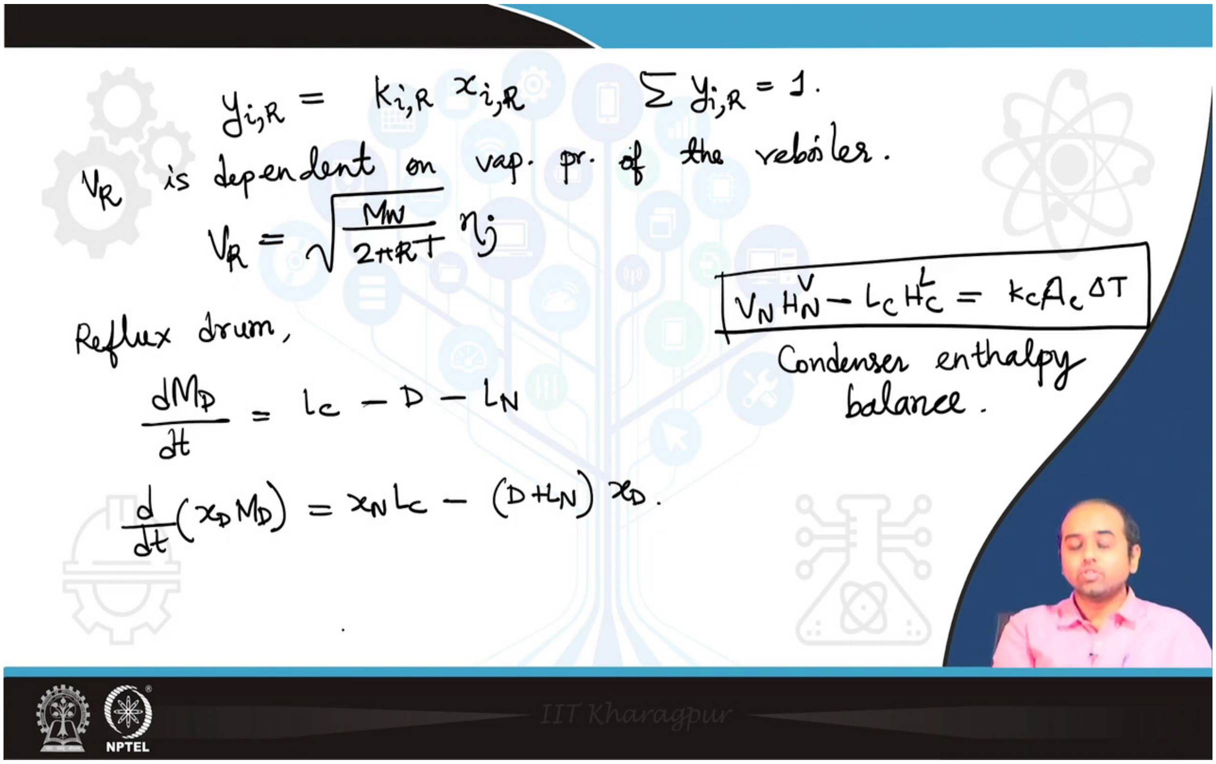

$y_{i,R} = k_{i,R}\, x_{i,R}$ $\qquad \sum y_{i,R} = 1.$

$V_R$ is dependent on vap. pr. of the reboiler.

$$V_R = \sqrt{\frac{M_W}{2\pi R T}}\, \eta_j$$

Reflux drum,

$$\frac{dM_D}{dt} = L_C - D - L_N$$

$$\frac{d}{dt}(x_D M_D) = x_N L_C - (D + L_N)\, x_D.$$

$$\boxed{V_N H_N^V - L_C H_C^L = k_C A_C \Delta T}$$

Condenser enthalpy balance.

And this is this holds are the reboiler, this also holds at the reboiler. Now, this VR the volumetric flow rate at the reboiler is dependent as I was seeing that this is something which you cannot calculate from the enthalpy balance for the Vj's. So, this VR is dependent on the vapor pressure in the reboiler. So, VR is essentially something like this, considering it to be an ideal gas this is the sort of the vapor pressure in the system.

Similarly, we can also work out the reflux drum, so the reflux drum, the liquid flow rate from the drum d minus Ln. Similarly, d dt of the component flow rates can also be written down as xn Lc minus d plus Ln. Now, what is this L, I mean this Lc the flow rate is something that you can calculate it out from the enthalpy balance of the total considering it to be a total condenser in that case, isn't it?

So, the total difference or the total vapor component that is actually condensed or the total heat capacity is what Vn HNV minus Lc HCL this is equal to Kc AC sort of LMD something, isn't it? Or the net delta T or whatever you can consider for the condenser this is the condenser enthalpy balance, this is for the condenser heat balance.

So, from the condenser this heat that is exchanged in the condenser you can calculate out what is the liquid flow rate Lc from that problem and then you substitute and get you the dynamics of the reflux term as well as already looked into how the dynamics of the reboiler is important.

Now, as I have said so, this is how the overall picture of the multistage multicomponent batch distillation process, I have tried in the beginning to emphasize the motivation for the batch system and also please note that this just came to my mind at the end that in a continuous distillation process in the beginning there is always a batch process or startup time. So, if during the startup phrase, it is essentially a batch process.

So, the startup of the continuous reactor is also something modelled in the form of the batch distillation process or in the same way, where the dynamics is important, we also calculate out what is this you know this the startup phase or the dynamic phase of the continuous distillation column and is the same framework that we have just seen for the batch process where the dynamics is important and it is not in a steady state.

So, the startup of the continuous reactor can also be thought about as a batch process and this is something where the calculations are also very relevant. So, with this I think, I will close this lecture today, I hope all of you liked this class on the batch distillation process and you understood or realized the dynamics of the batch process which is relevant not only for batch type of distillation, but also in the case of content startup phase of the continuous distillation column. Thank you hope you liked this lecture.