Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 31
Modelling of multistage distillation process

Hello everyone we are going to learn about modelling the multi-stage distillation process in this week, of course, I believe it will also extend to the next week. Now, distillation all of you knew is the separation of two or more species based on the difference of the relative volatilities. Now, in distillation the major calculation or the major process calculation involves the calculation of the number of stages as well as the stage compositions.

Now, I am sure all of you have already studied the classical McCabe-Thiele theory method or the Ponchon-Savarit method in your mass transfer class. So, here we are going to talk about or take a more rigorous approach towards how the stage calculations can be done using a computer program and this is applicable for more than one species, I mean all of you know that in the McCabe-Thiele method it is for a binary system and then the other assumptions are there the constant molar overflow and all those things.

So, these are not realistic assumptions or these are not something which we observe or see in practice. So, to have a more rigorous approach there are several calculation types or methods which is generally implied and each one of them has their own merits or demerits and this is something which is widely adopted in the commercial process simulators, for example, Aspen plus.

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CONCEPTS COVERED

- Degree of freedom analysis
- Flash distillation
- Rachford-Rice method of convergent solution

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So, first let us look into the this degree of Freedom analysis for a simple flash process and then for, from there we will talk about the Rachford-Rice method and this is something which is relevant for a flash distillation and then slowly we will move on to the, these multi-stage columns and we will see the different methods of calculation as well as strategies to calculate the tray compositions for multi component multi-stage process.

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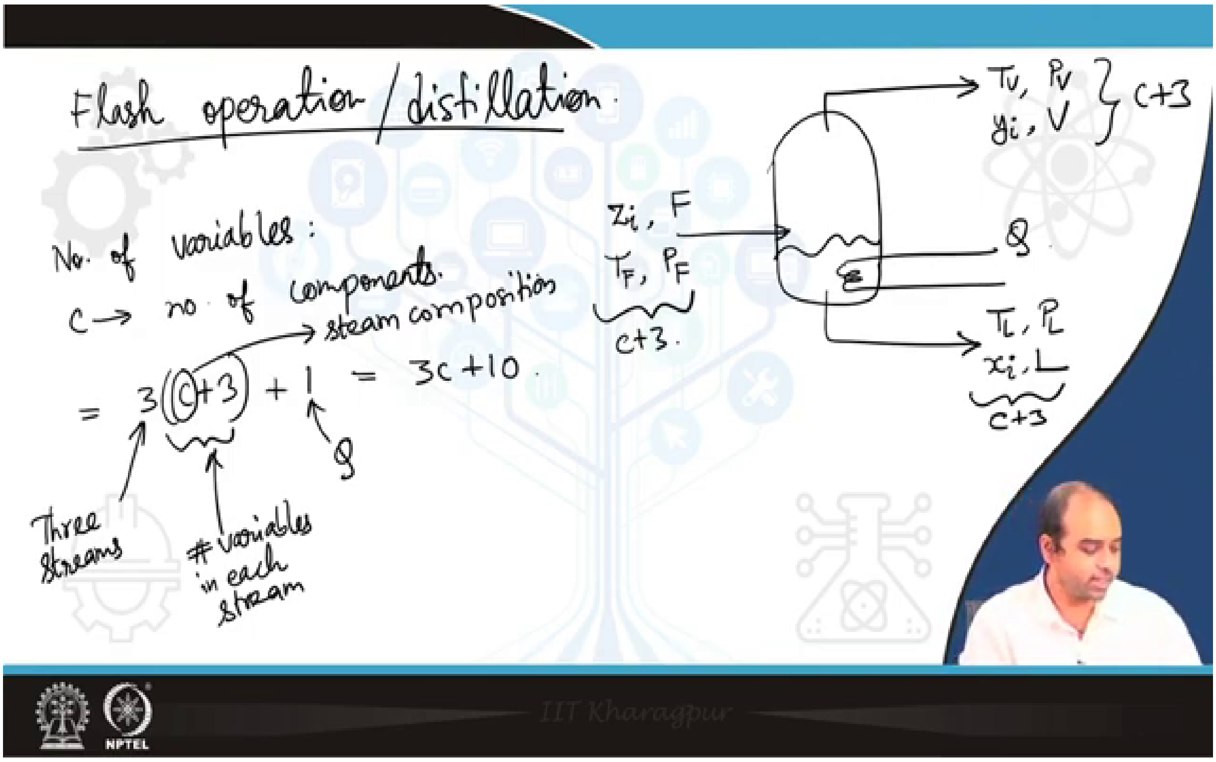

Flash operation / distillation

No. of variables :

$C \rightarrow$ no. of components.

$$= \underbrace{3}_{\text{Three streams}}(\underbrace{\overset{\text{steam composition}}{\boxed{C}}+3}_{\text{\# variables in each stream}}) + \underbrace{1}_{Q} = 3C+10.$$

So, now for a flash distillation, flash is something which is equivalent to a single stage in a multi-stage process. So, flash operation or flash distillation let us try to have a clear picture on the degrees of freedom for this flash case and this will slowly help us to understand the degrees of freedom later on for a multi-stage process.

So, this is a flash drum, the feed then you have one top and one bottom streams and let us say that there is some external amount of heat supplied for this flash process. So, let us write down the flash composition as Z i so i represents the component fraction then F is the feed flow rate, T F is the temperature of the feed, P F is the pressure of the feed.

Let me also write down the top and the bottom string variables. So, the pressure of the top stream is written as TV and then pressure as PV and we write the top composition as y i and the flow rate of the top string is V. Similarly, for the bottom stream is the liquid and the pressures are TL, PL this generally the liquid stream and the top is mostly the vapor stream, x i and liquid flowrate is given as L.

So, what are the number of variables in this simple flash process? So, if we do a variable count where C is the let us say the number of components in this process. So, we have from the stream, from the stream, a feed stream side we have C plus 3 number of variables I mean there are C plus 3 number of variables in all the streams.

So, the total number of variables is 3 times the feed the top and the bottom streams, C plus 3 number of variables and there is 1 extra variable which is the Q or the external heat. So, total you have 3 C plus 10 number of variables. So, this is corresponding to 3 streams and this is for each number of components, number of variables in each stream. And this C actually is from the stream composition. So, this is clear to all of you, we have in a flash total C, 3 C plus 10 number of variables.

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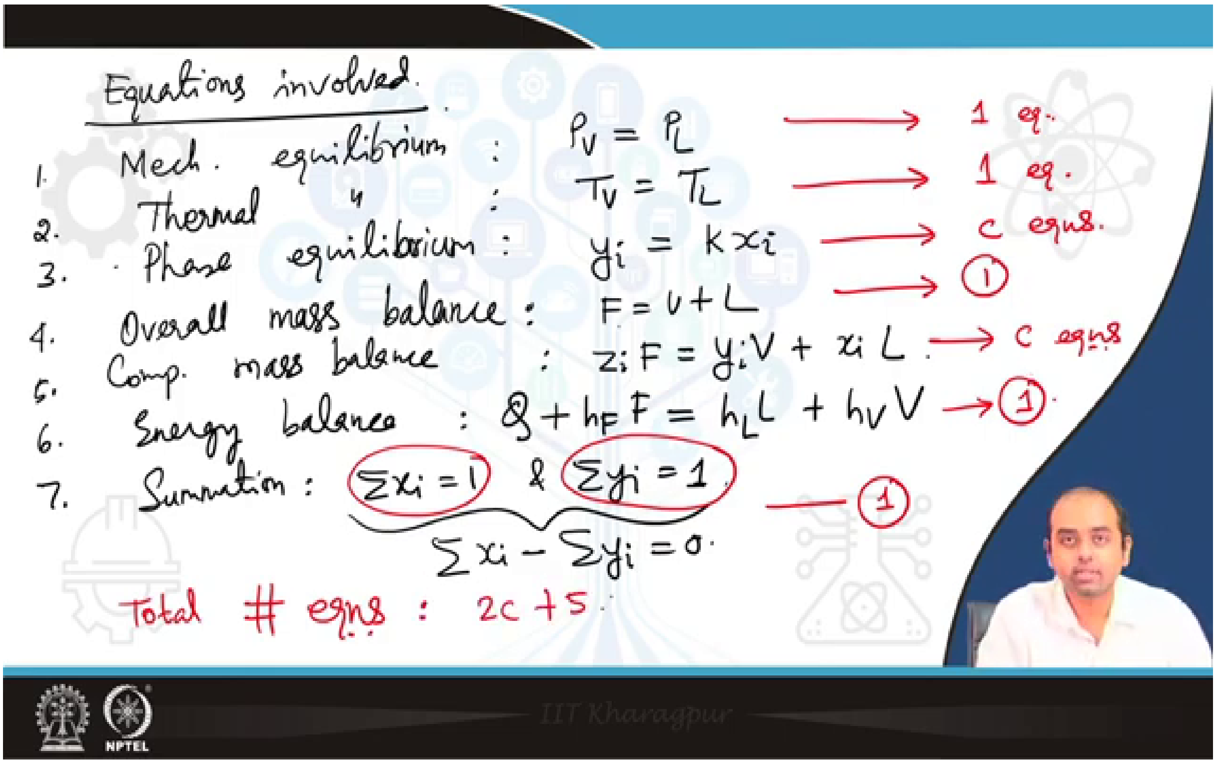

Equations involved.

1. Mech. equilibrium : $P_V = P_L$ → 1 eq.
2. Thermal " : $T_V = T_L$ → 1 eq.
3. Phase equilibrium : $y_i = K x_i$ → C eqns.
4. Overall mass balance : $F = V + L$ → ①
5. Comp. mass balance : $z_i F = y_i V + x_i L$ → C eqns
6. Energy balance : $Q + h_F F = h_L L + h_V V$ → ①
7. Summation : $\boxed{\sum x_i = 1}$ & $\boxed{\sum y_i = 1}$ — ①

$$\underbrace{\sum x_i = 1 \quad \& \quad \sum y_i = 1}_{\sum x_i - \sum y_i = 0}$$

Total # eqns : 2C + 5.

Now, let us look into the equations involved in this batch calculation, sorry, in this flash calculations, equations involved. So, the first equation we have is mechanical equilibrium, so which means the pressure of the vapor stream is equal to the pressure of the liquid stream that has to be satisfied. Similarly, thermal equilibrium, so it means TV is equal to TL, then you also have phase equilibrium. So, this is in chemical equilibrium that is why all three are also balanced.

So, we know the phase equilibrium relationship as y i this is true for all components K x i, K is the constant, then we have the overall material balance or mass balance, so that is F is equal to L plus, V plus L. Then we have the component mass balance, so that is Z i F is equal to y i V plus x i L.

Then we have the energy balance so which is Q plus h F, so this is enthalpy in, and minus enthalpy out so h L L plus h V V. Then we have the summation equation. So, please note the summation equation could be sigma x i is equal to 1 and sigma y i is equal to 1, so there could be two summation equations but since we already have the overall mass balance and the component mass balance for all the components then it is this, these two can be reduced to one equation, because one is already taken care of. I mean just let me tell you the number of equations we are getting for each case.

So, this gives you one equation, this gives you one equation, this has C equations for C number of components, this is 1 equation, this is again C equation. Now, please note that if you are considering the overall mass balance as well as the component mass balance. So, when we try to write down the summation equation for one of the cases is already accounted for because summation of all the individual component flow rates will give you the summation of the total flow rate, either liquid or vapor or feed stream.

So, one of them, so either you consider two individual summation equations for the liquid and the vapor fraction and you do not consider overall mass balance or one of the, the last component balance can be ignored because the last can be written down as 1 minus of the rest of the components or you consider only one of the summation equations.

So, if you are considering C number of species balance equation then from the summation equations we are only getting 1 equation and energy is 1. So, the total number of equations that we are getting total number of equations we are getting is 2 C plus 5, 2 C plus 5 number of equations.

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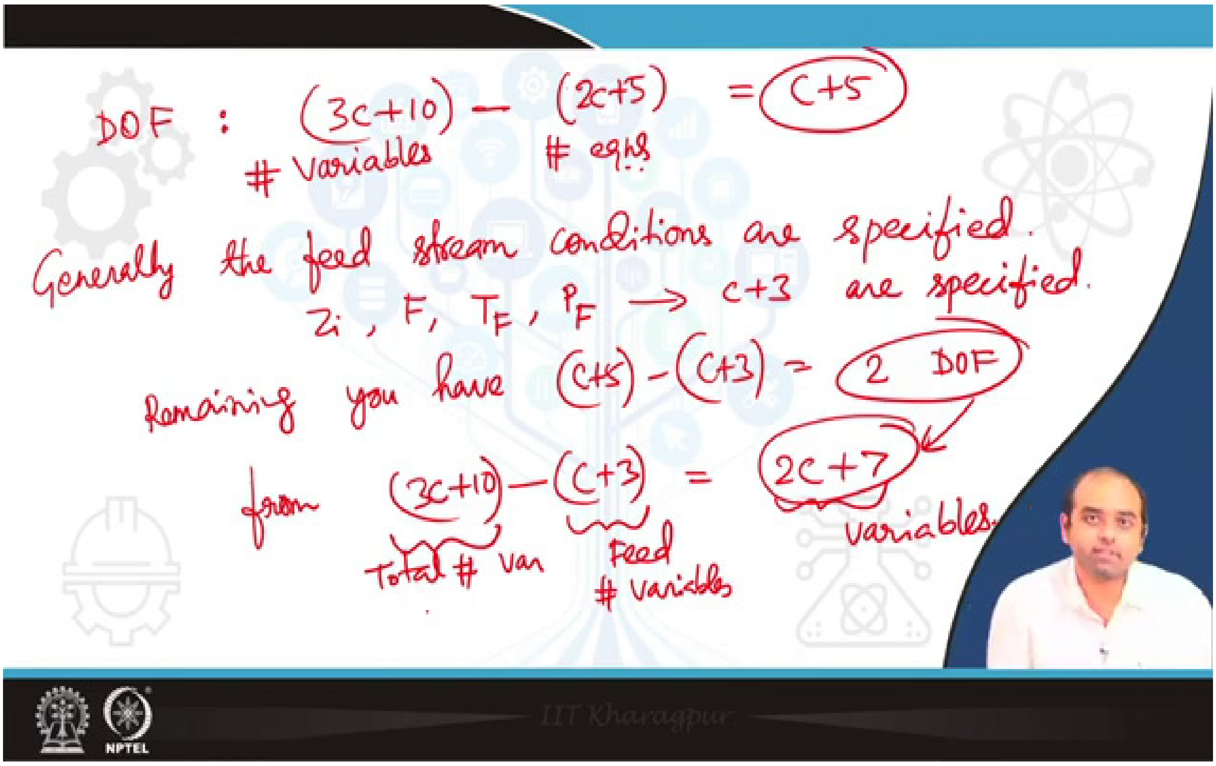

$$\text{DOF}: \underbrace{(3c+10)}_{\#\text{ variables}} - \underbrace{(2c+5)}_{\#\text{ eqns}} = \boxed{C+5}$$

Generally the feed stream conditions are specified.

$Z_i, F, T_F, P_F \rightarrow c+3$ are specified.

Remaining you have $(C+5)-(C+3) = \boxed{2 \text{ DOF}}$

from $\underbrace{(3c+10)}_{\text{Total \# var}} - \underbrace{(C+3)}_{\text{Feed \# variables}} = \boxed{2c+7}$ variables.

So, what is the degree of freedom of the problem? So, degree of freedom in this problem is you are having 3 C plus 10 number of variables since this is the number of variables you have for the flash problems and you have 2 C plus 5 number of equations, this is the number of equations you have.

So, total you are getting C plus 5 as the number of variables in the system, now, sorry degrees of freedom in the problem. So, which has to be specified for a unique problem. Now, if generally the stream, the feed stream conditions are specified in a problem, generally the feed stream conditions are specified because you know what is the feed to your system. So, what are the feed components? Z i, F, T F and P F, these are the feed compositions. So, C plus 3 are specified.

So, remaining from this C plus 5, so remaining you have C plus 5 minus C plus 3. So, that is 2, so 2 degrees of freedom have to be specified from the problem conditions. So, two conditions have to be specified from, so this is the total number of variables and this is the feed number of variables, so which means you are having 2 C plus 7 number of variables to be specified. So, two degrees of freedom have to be specified from this 2 C plus 7 number of variables. Now, let us look into the possible scenarios what could be the possible scenarios of the specification and accordingly what kind of process or what kind of outputs do you get.

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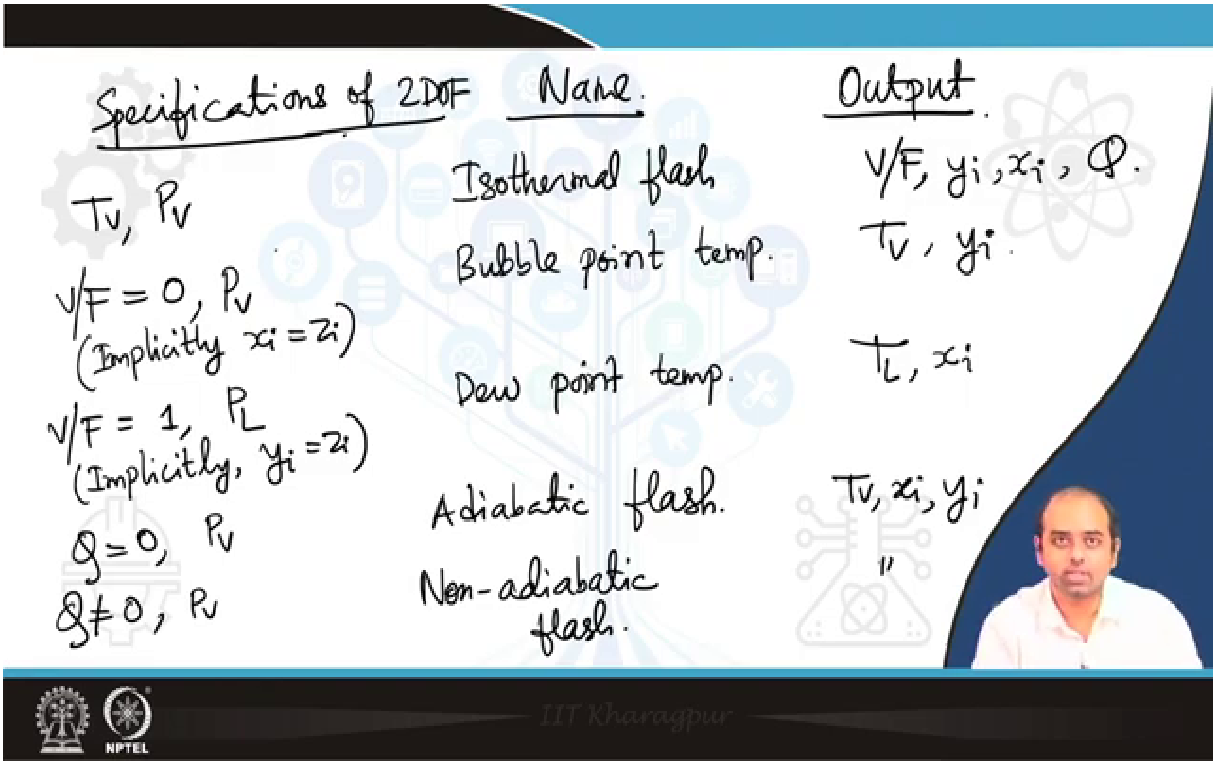

Specifications of 2DOF	Name.	Output.
T_V, P_V	Isothermal flash	V/F, y_i, x_i, Q.
$V/F = 0$, P_V (Implicitly $x_i = z_i$)	Bubble point temp.	T_V, y_i.
$V/F = 1$, P_L (Implicitly, $y_i = z_i$)	Dew point temp.	T_L, x_i
$Q = 0$, P_V	Adiabatic flash.	T_V, x_i, y_i
$Q \neq 0$, P_V	Non-adiabatic flash.	"

So, if the specification let us list it down, is, we have specifications and then what is the name of the corresponding process that we generally call and what is the output. So, if the temperature of the vapor stream or the pressure, both temperature and vapor streams are specified then we call that process to be isothermal flash.

So, in this case the typical output is the total top flow rate, then that of composition, bottom composition, Q. So, if you specify the V plus F to be equal to 0, so there is no vapor fraction and the pressure, so this is the bubble point temperature, so from here with the typical outputs that we get is T V, then y i. So, this of course means that this implicitly means x i is equal to Z i there is everything is in liquid state.

Similarly, V by F could be equal to 1 and as yes and then we specify the liquid temperature, so this implicitly means that everything is in vapor phase, this is called dew point, please note the dew point temperature is more for, more than the bubble point temperature. So, bubble point is the temperature at which the first vapor drops starts to form and dew point is the temperature at which all the vapor I mean the first condensate starts to form.

So, in this case we have the T L and the x i. Similarly, you can also set Q to be equal to 0, Q is also one of the perimeters, parameters and P V the pressure in the vapor phase, so this is called adiabatic flash, no external heat, so typically the outputs are T V, x i, y i. Then also you can specify your non-zero Q and P V so this in this case Q has to be specified is not zero, so it is non-adiabatic flash, and this is the same term.

So, these are the possible different scenarios that can occur depending on the specification of the two variable, specification of two degrees of freedom in this flash process. So, now let us look into the situations or looking to the calculations for what happens when we have isothermal flash and when we have adiabatic flash.

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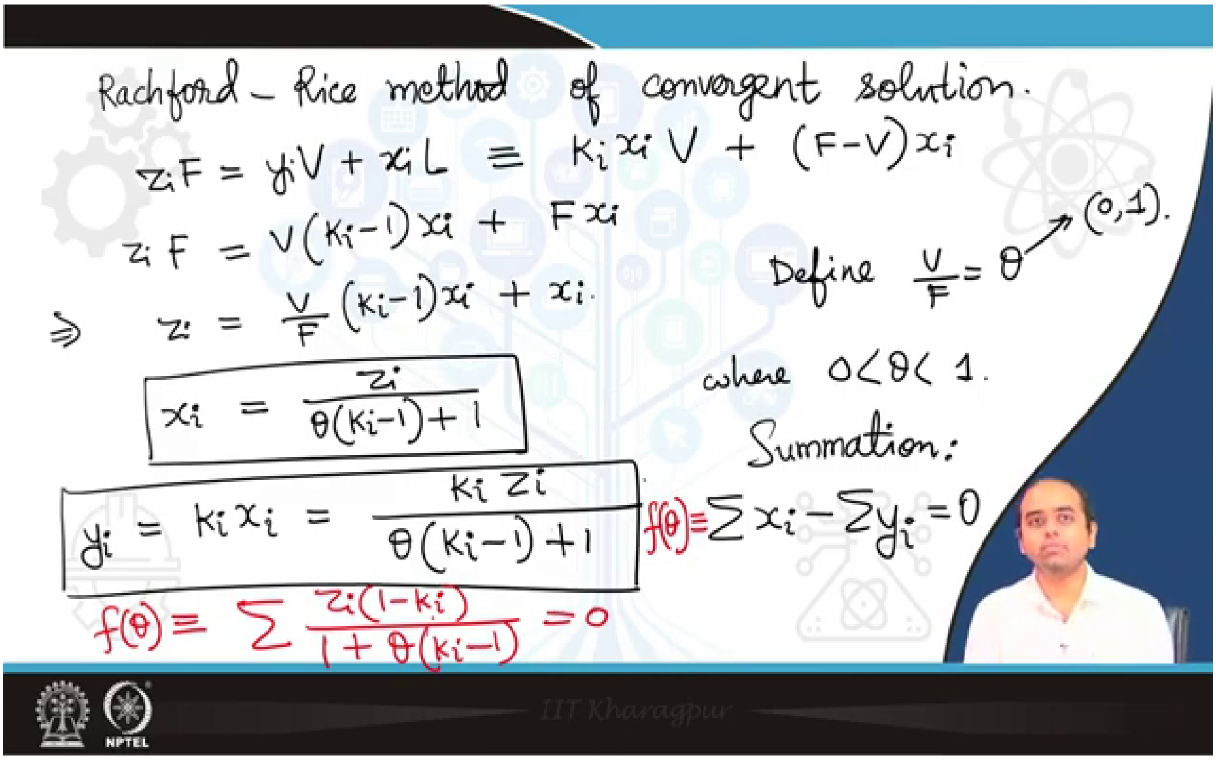

Rachford – Rice method of convergent solution.

$$z_iF = y_iV + x_iL \equiv K_ix_iV + (F-V)x_i$$

$$z_iF = V(K_i-1)x_i + Fx_i$$

$$\Rightarrow z_i = \frac{V}{F}(K_i-1)x_i + x_i.$$

Define $\frac{V}{F} = \theta \rightarrow (0,1).$

where $0<\theta<1.$

$$\boxed{x_i = \frac{z_i}{\theta(K_i-1)+1}}$$

$$\boxed{y_i = K_ix_i = \frac{K_iz_i}{\theta(K_i-1)+1}}$$

Summation:

$$f(\theta) \equiv \sum x_i - \sum y_i = 0$$

$$f(\theta) \equiv \sum \frac{z_i(1-K_i)}{1+\theta(K_i-1)} = 0$$

So, this process of estimating all the compositions for a simple flash distillation is generally is proposed by Rachford-Rice, so we look into the Rachford-Rice method of convergent solution. Please note here we are talking about multi-component systems, so had it been a binary system you could have easily calculated out just by simple substitution but for multi component it is not so straightforward, you need an iterative solution.

So, the first equation that we have is the species balance, overall species balance. So, this is the, and this can also be written down as K i, y i can be written down from the phase equilibrium K i x i and V, and L can be written down as F minus V, I am just trying to write down minimizing the number of unknown variables. So, this can be effectively written down as V into K i minus 1 x i Plus F x i, so this is Z i into F and correspondingly I can further write it down as Z i is equal to V by F K i minus 1 x i plus x i.

So, if I define, so if I try to define this fraction like V by F to be equal to theta where theta is always in between 0 and 1. So, I can write substitute, instead of writing in terms of Z i I can write x i as Z i by theta into K i minus 1 plus 1 so this is the equation I am having, where of course, theta is in between 0 and 1 so that is a fraction.

Similarly, I can also write y i as equal to K i x i so this is equal to K i the top equation, this is something I can write for the Y i also. Now, please note the summation equation. So, we already written down the summation equation which is summation of sigma x i minus summation of y i is equal to 0. So, let us call this equation, this as f of theta because theta is the only unknown in this problem, let us define this equation or the summation equation as the form of f of theta, let me write in a different colour, so it is more visible.

Because in this equation the summation equations Z i I mean what the summation equation looks like? I can merge them these to, so this is the summation equation I am having. So, please note that in the summation equation Z i is the feed composition that is known, K i is known from the thermodynamics, so K i is the vapor liquid equilibrium constant and that is from the thermodynamics you have several of these thermodynamic relations which can helps you to compute these phase equilibrium constant, vapor liquid equilibrium constant, you have those Van Laar models, UNIQUAC, UNIVAC which can help you to calculate these constants and typically K is a function of temperature and pressure in the system.

So, it is not that temperature is not defined for this problem this K i is T is actually dependent on the temperature and pressure of the system that is maintained. So, temperature and pressure are something which determines this case.

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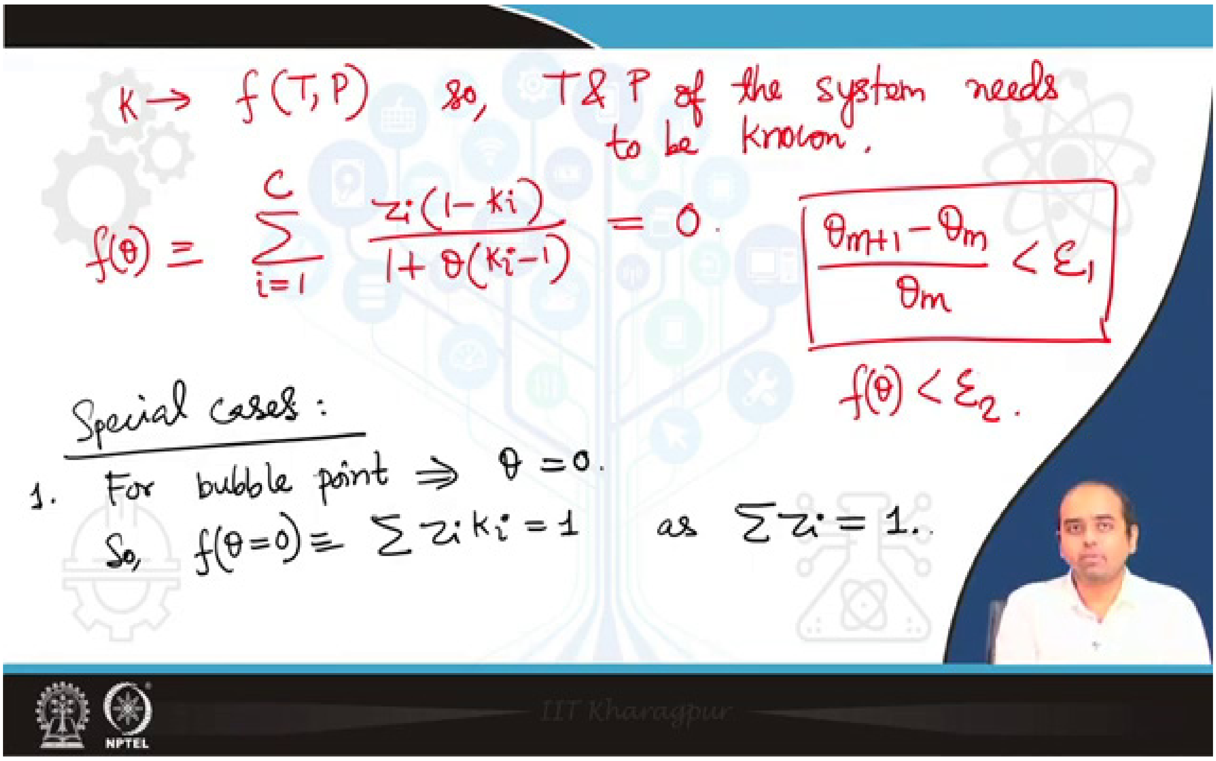

K → f(T, P) so, T & P of the system needs to be known.

$$f(\theta) = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\theta(K_i-1)} = 0.$$

$$\boxed{\frac{\theta_{m+1}-\theta_m}{\theta_m} < \varepsilon_1}$$

$$f(\theta) < \varepsilon_2.$$

Special cases :

1. For bubble point ⇒ $\theta = 0$.
So, $f(\theta=0) = \sum z_i K_i = 1$ as $\sum z_i = 1$.

So, let me write it down in this case K is a function of temperature and pressure. So, T and P of the system needs to be known and then only you will have this f of theta which is the summation and summation is across all the components can be worked out. So, this is the iterative solution you have, so what is the unknown, unknown is the theta, so essentially you have to choose a theta and then work out that solution I mean the summation equation and see whether it is close to 0 or not.

If not then it is something that has to be again reiterated with the new guess so you choose a theta and you continue to, continue this iteration as long as the relative error between two successive iterations of this theta is less than this tolerance value you do not stop. So, until the theta is, the theta that you obtain in this step and the subsequent step is below, relatively below tolerance limit as well as f of theta also needs to be satisfied, f of theta also needs to be satisfied below a certain tolerance.

So, let us say this could be epsilon 1, this could be epsilon 2 where we set this I mean theoretically it is not possible to get 0 but it is a very small number you can set and f of theta should be below 10 to the power minus 3 or minus 6 whatever, and this above condition is also specified that changing the iteration or changing with the different new guesses of theta you do not get, I mean that is not changing in this calculation and f of theta is also very small quantity, so you can say that this is a converged solution and this is acceptable because theta is not changing with the iterations.

Now, what are the possible special cases? So, one of the special case is for bubble point, theta is equal to 0. So, from this f of theta equal to 0 you get summation of Z i K i is equal to 1, is not it as summation of Z i is equal to 1. So, from here at the bubble point you can work out or you can find out what are the different K i's of the system from this definition that summation of Z i K i is has to be equal to 0. And this setting this bubble point means you are already defining your temperature, either temperature or pressure in the problem, so the other unknown temperature pressure which is a function of this K i can be worked out from there.

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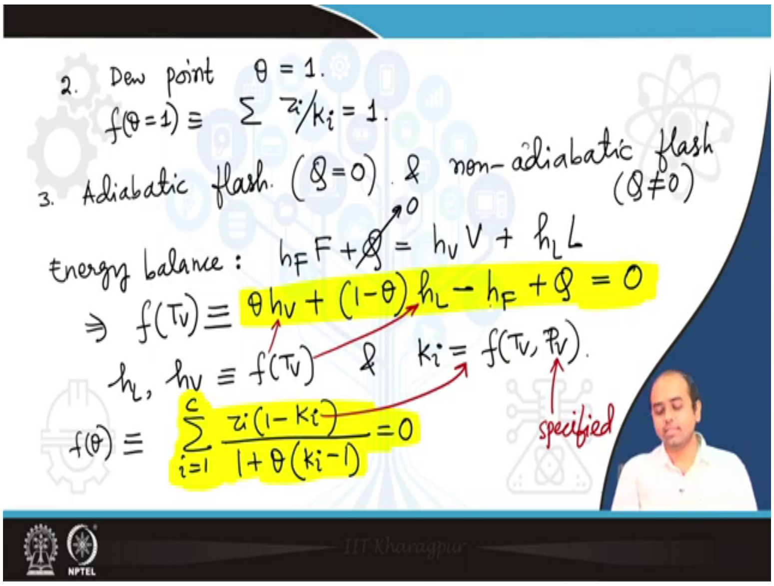

2. Dew point $\theta = 1.$

$f(\theta=1) \equiv \sum z_i/k_i = 1.$

3. Adiabatic flash $(Q=0)$ & non-adiabatic flash $(Q \neq 0)$

energy balance : $h_F F + \cancel{Q}^{\,0} = h_V V + h_L L$

$\Rightarrow f(T_V) \equiv \theta h_V + (1-\theta) h_L - h_F + Q = 0$

$h_L, h_V \equiv f(T_V)$ & $k_i = f(T_V, P_V)$

$f(\theta) \equiv \sum_{i=1}^{c} \frac{z_i(1-k_i)}{1+\theta(k_i-1)} = 0$

specified

So, the second scenario is in the case of the dew point. So, if you have dew point then there is no liquid fraction, everything is in vapor state. So, theta is equal to 1, so f of theta is equal to 1, this equation now gets converted to sigma of Z i by K i is equal to 1, I mean you can work out the individual steps.

So, here I mean, if you initially, I mean since here the pressure would be specified or that is generally the case, so K i is a function of temperature and pressure. So, if the pressure is specified so in this equation only the temperature will be unknown and so from here you can calculate the dew point temperature and I hope all of you realize that how do we get this equation, this is for the case when theta is equal to 1.

Next is the case of adiabatic flash. So, when you have adiabatic flash our equations so far does not involve the use of Q. So, how this Q will be taken into account is that for this Q or the for making the energy balance you have to write the enthalpy balance here. So, let us write down the energy balance first. I mean this is also true for adiabatic and non-adiabatic flash.

So, let us make this general, so this is the scenario when we have Q specified in this problem, whether it is zero or non-zero that is a separate thing but when Q is specified as one of the degrees of freedom, this is how we write down this additional equation. So, this h V, h L are essentially all functions of temperature.

So, if I just do this V by F so I can get theta h V, let us say Q is setting to 0 for the case of adiabatic h V plus 1 minus theta h L minus h F plus Q you will be having. So, this is the equation we are getting where h L, h F so generally h L, h V these are all functions of T V and K i is a function of T V and PV. So, this is instead of I have not written down as functions i because we do not know what is the exact functionality of this enthalpy of the specific heat of the enthalpy with respect to temperature, but we know that it is related to the temperature.

So, essentially in this equation theta h V this equation that we are seeing here, this equation that we are looking here has only the unknown of T V because these specific heats of the enthalpies are dependent on the temperature T V and we already have that f of theta equation. So, for the theta which is also an unknown, we already have this equation is f of theta.

So, together please note that in this equation also the K i which is present is a function of T V and P V so even in the, this flash condition the pressure will be specified and so this T i, sorry, so this K i, this K i is a function of temperature and pressure and since pressure is generally specified. So, here also in this equation temperature is unknown. So, in these two equations you are having theta unknown and temperature as the unknown, so for two unknowns you have two equations which again needs to be solved iteratively for two variables now, the previous one was the case of only one unknown variable and it is a non-linear equation sort of nonlinear equation.

Here also as you insert the functionality of the specific heats of the enthalpy as a function of temperature this equation will also become slightly non-linear, so you have two non-linear algebraic equation which needs to be solved out in a coupled way because there are two unknowns. Of course, you can substitute one of the unknowns from that equation to here but essentially these are two algebraic equation, non-linear algebraic equation which needs to be solved out and then you will get the values of theta and your K i.

So, here this say, as I said this is a function of T V, this is a function of T V, h F is known, a known quantity. So, this is the method of convergent or the Rachford-Rice method of convergent solution for a batch process. So, with the same idea we will extend towards the multi component multi-stage process, so batch is a simplest one with the case of only single stage, but this is how you generally do the calculations for multi component systems, the same idea will be explored and will be extended for the case of the multi component system.

So, in the next lecture we will first try or work or discuss on the shortcut method which is based on the Fenske Underwood and Gilliland correlations and then we will move into this rigorous calculation methods of multi component multi stage processes. I hope all of you had a fair understanding of this degree of freedom analysis in this class, as well as how the Rachford, this method of Rachford Rice is used for multi component separation in a flash distillation process. I hope all of you found this useful, thank you.