Process Control and Instrumentation

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Lecture - 5
Mathematical Modeling (Contd.)

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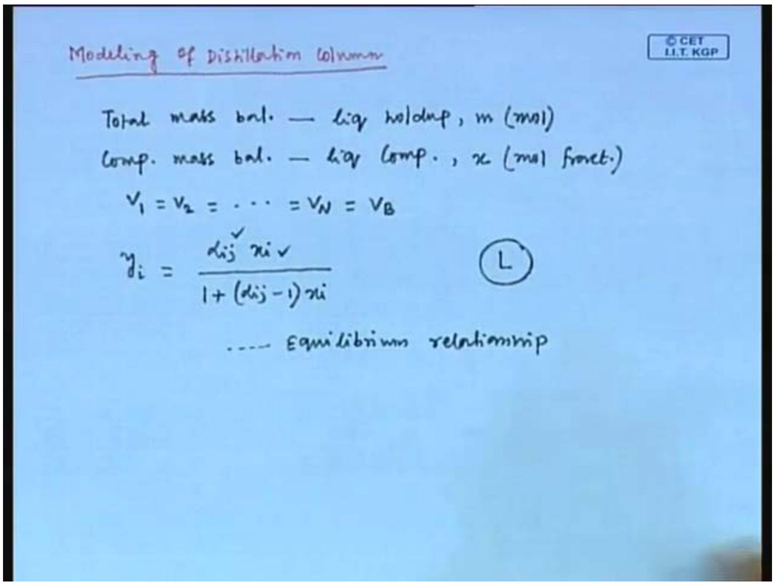

Modeling of Distillation Column

Total mass bal. — liq holdup, m (mol)

Comp. mass bal. — liq comp., x (mol fract.)

$V_1 = V_2 = \cdots = V_N = V_B$

$$y_i = \frac{\overset{\checkmark}{\alpha_{ij}} x_i \checkmark}{1 + (\alpha_{ij} - 1) x_i} \qquad \textcircled{L}$$

---- Equilibrium relationship

Today, we will continue our discussion on modeling of distillation column. So, in the last class, we have derived mass balance equations, I mean first, we have derived total mass balance equation along with the component mass balance equation fine. Now, we have mentioned that the total mass balance equation is use to calculate liquid holdup represented by m, unit is suppose mole and component mass balance equation, we can use to calculate liquid composition, which we have represented by x and x is the mole fraction. And based on some assumptions, we have concluded that all vapor flow rater are identical that means, V 1 equals to V 2 equals to V N equals to V B.

Now, other variables, I mean apart from these variables include the vapor phase composition fine. Another one is liquid flow rate, we have discussed the calculation procedure of vapor flow rate of any component i, that is y i equals to alpha i j x i divided by 1 plus alpha i j minus 1 into x i. This equation, we have derived and this is called as equilibrium relationship our assumption is that alpha i j remains constant throughout the column. So, alpha i j is known, x we can get from the component mole balance equation or component mass balance equation, so we can calculate the vapor composition.

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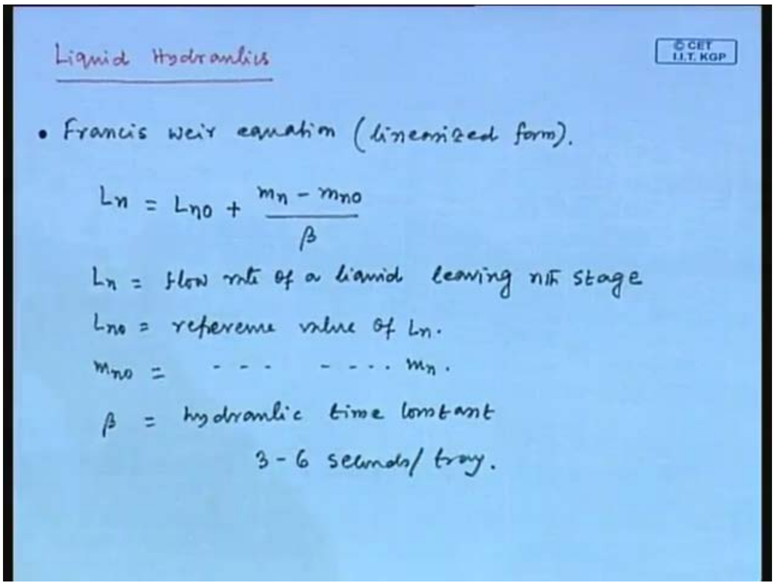

Liquid Hydraulics

- Francis weir equation (linearized form).

$$L_n = L_{n0} + \frac{m_n - m_{n0}}{\beta}$$

L_n = flow rate of a liquid leaving nth stage

L_{n0} = reference value of L_n.

m_{n0} = - - - - - - - m_n.

β = hydraulic time constant

3 - 6 seconds/tray.

Today, we will discuss the calculation of this liquid flow rate that means, we will discuss liquid hydraulics. The liquid hydraulics is calculated by the use of well known Francis weir equation, liquid flow rate is calculated by the use of well known, Francis weir equation. So, for the example distillation column, we will consider the simplified form of this Francis weir equation and that is the linearised form.

So, we will consider the linearised form of Francis weir equation. So, if L n is the flow rate of a liquid, leaving n-th stage then the Francis weir equation correlates, L n equals to L n naught plus m n minus m n naught divided by beta. This is the Francis weir form Hoyer L n is the flow rate of a liquid steam, flow rate of a liquid steam, leaving n-th stage, L n naught is the reference value of L n. Similarly m n is the reference value of sorry, m n naught is the reference value of m n, another term is included in the Francis weir formula that is beta, beta is hydraulic time constant.

The value of beta is typically, taken in between 3 to 6 minutes, the beta is taken in between 3 to 6 naught minute seconds or each tray. So, beta is the hydraulic constant it is typically, 3 to 6 seconds for each tray that means, you see the difference between m n and m n naught, that is divided by the hydraulic time constant then that amount is included with L n naught to calculate the L n. This is the simplified version of Francis weir formula, other forms include the non-linear versions basically.

So, we will consider this amplified form in the example distillation column modeling, now this is all about the distillation model. So, the model includes basically, the mass balance, I mean total mass balance, component mass balance then the vapor flow rates, which are identical for all trays equilibrium relations have to calculate the vapor phase composition and last one is the tray hydraulics for the calculation of liquid flow rates fine. Now, we will use this model to analyze the degrees of freedom.

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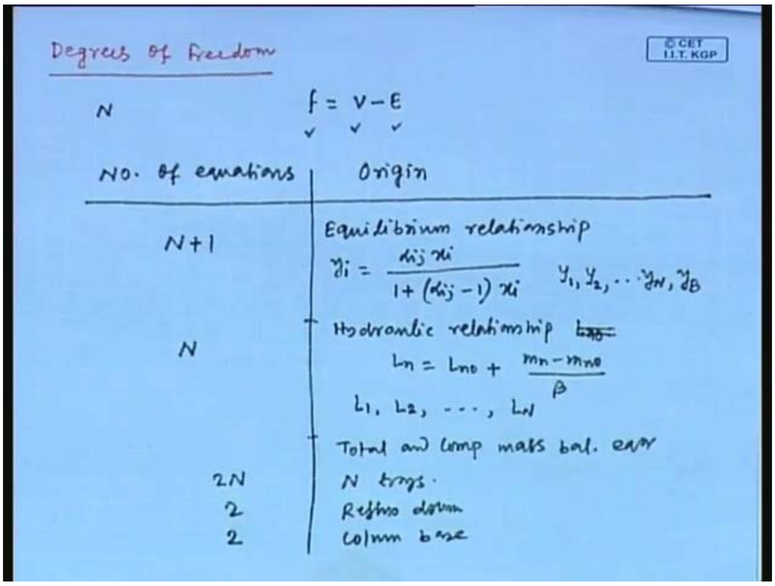

Degrees of Freedom

N

$f = V - E$
✓ ✓ ✓

No. of equations	Origin
N+1	Equilibrium relationship $y_i = \frac{\alpha_{ij} x_i}{1 + (\alpha_{ij} - 1) x_i}$ $y_1, y_2, \ldots y_N, y_B$
N	Hydraulic relationship ~~L_{no}~~ $L_n = L_{no} + \frac{m_n - m_{no}}{\beta}$ $L_1, L_2, \ldots, L_N$
	Total and comp mass bal. eqn
2N	N trays.
2	Reflux drum
2	Column base

So, the next topic is the degrees of freedom, for the example distillation degrees of freedom. Now here, we will consider one example although, we have consider for the in the development of the distillation model that is N, N is basically the number of trays excluding condenser and reboiler, will use this nomenclature we will use this notation in the degrees of freedom analyses. So, you can recall the degrees of freedom represented by f, which is correlated with V and E by this form, f is the degrees of freedom, V is the number of independent process variables and E is the number of independent equations.

So, to calculate the degrees of freedom, we need to find both and E for the example distillation column. So, first we will go for the number of equations calculations, number of equations and the origin of there those equations will first discuss this part. So, first one is a equilibrium relationship what is the equilibrium relationship, we have consider for the example column, that is y i equals to alpha i j x i divided by 1 plus alpha i j minus 1 into x i.

So, how many y, we need to calculate, how many y are involved in the distillation model y 1 y 2 y n another y is involved, that is y b, the composition of boiled a vapor. So, what is the number N plus 1. So, total number of equilibrium equations involved in the distillation model is N plus 1.

Next is hydraulic relationship that is L n naught equals to sorry, L n equals to L n naught plus m n minus m n naught divided by beta. How many liquid flow rates are involved in the distillation model L 1 L 2 up to L n, n number of liquid flow rates, we have to calculate using this Francis weir formula, we cannot consider the distillate flow rate and bottom flow rate although those are liquid flow rates, because those are not calculated by the employment of this Francis weir equation.

So, total number of equations N, next is component and total mass ablation equations, total and component mass balance equation, how many component and total mass balance equations are involved. First we will consider for N number of trays for N number of trays, how many equations are there, 2 N one total mass balance equation, one component mass balance equation for each tray that means, 2 equations for each tray. So, for N number of equations, N number of stages, we have 2 N equations.

Next, we will consider for the reflux drum number of equations to similarly for the column base, number of equations 2, one component and another one total mass balance equations. So, total number of equations how many.

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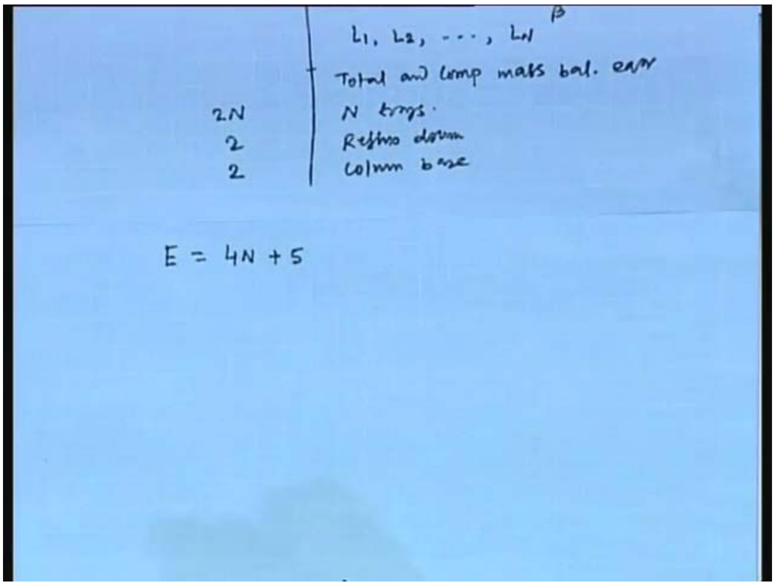

β

	$L_1, L_2, \ldots, L_N$
	Total and comp mass bal. eqn
$2N$	N trays.
2	Reflux drum
2	Column base

$E = 4N + 5$

Total number of equations E that is equals to 4 N plus 5. So, next we have to find that total number of variables V.

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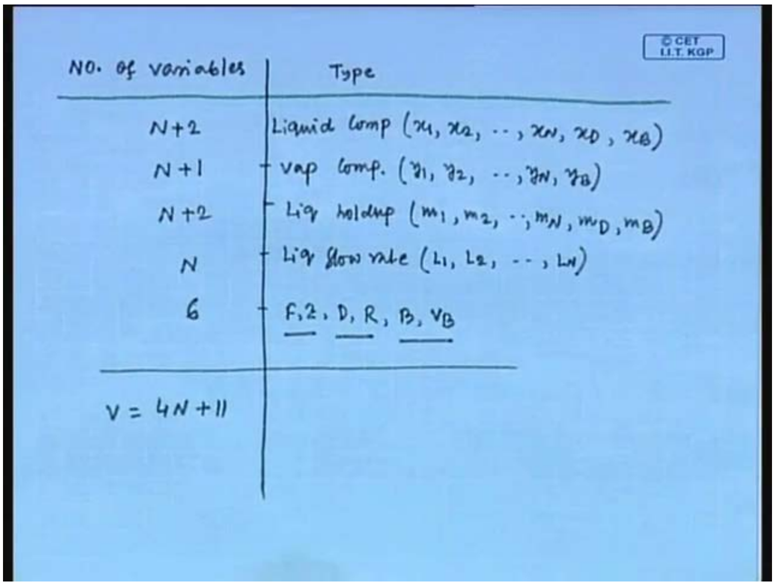

No. of variables	Type
$N+2$	Liquid comp $(x_1, x_2, \ldots, x_N, x_D, x_B)$
$N+1$	Vap comp. $(y_1, y_2, \ldots, y_N, y_B)$
$N+2$	Liq holdup $(m_1, m_2, \ldots, m_N, m_D, m_B)$
N	Liq flow rate $(L_1, L_2, \ldots, L_N)$
6	$\underline{F, z}, \underline{D}, R, \underline{B, V_B}$
$V = 4N + 11$	

Next, we will calculate number of variables and type of variables. So, first will consider the liquid composition, how many liquid compositions are involved x 1 x 2 x n, one for top section and one for bottom section, N number of liquid compositions N trays, one for reflux drum and one for column base. So, N plus 2 next vapor composition, how many vapor compositions are involved y 1 y 2 y n and one for column base, there is no vapor distillate, we have consider only the liquid distillate. So, 3 is no y D.

Accordingly, we have total N plus 1 equation, N plus 1 variable, those are vapor compositions. Next one is liquid holdups, one for each tray that means, m 1 m 2 up to m n, one for reflux drum and one for column base. So, N number of holdup for N trays and 2 for reflux drum and column base. So, total number is N plus 2.

Next one is liquid flow rates, how many liquid flow rates are involved L 1 L 2 L n, we are not including the flow rates of top and bottom products will consider those separately. So, total number of liquid flow rates N, now apart from this variables what are the other variables involved in the distillation modeling. First we will consider in the feed, what are the variables use for feed F and Z, what about top, I mean top section in the top section, we have another 2 variables. One is D, another one is reflux flow rate and what about the bottom section, one is bottom flow rate, another one is boil up.

So, this 2 are representing the feed, this 2 in the top section and this 2, we are considering for the bottom section, so how many then 6. So, V equals equal to how much 4 N plus 11, we got V equal to 4 N plus 5 and we have just calculated V equals to V equal to 4 N plus 11.

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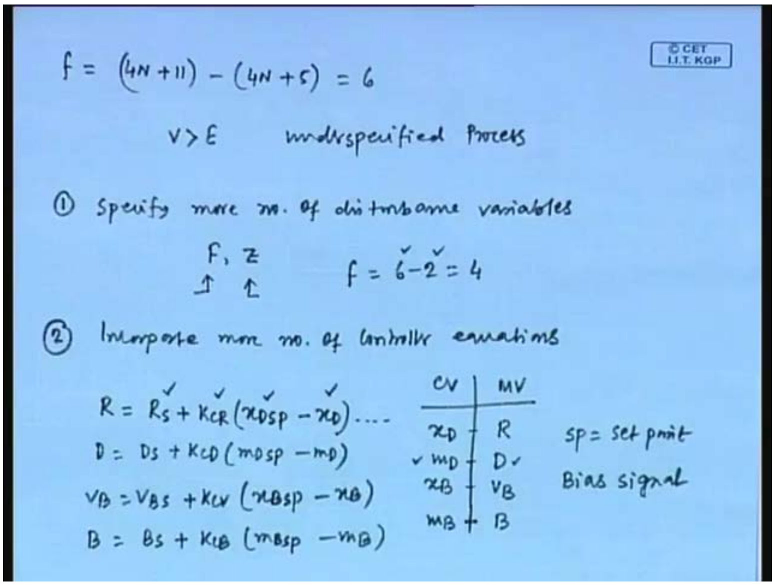

$$f = (4N + 11) - (4N + 5) = 6$$

$V > E$ underspecified Process

① Specify more no. of disturbance variables

$$\underset{\uparrow}{F}, \underset{\uparrow}{Z} \qquad f = \overset{\checkmark}{6} - \overset{\checkmark}{2} = 4$$

② Incorporate more no. of controller equations

$$R = \overset{\checkmark}{R_s} + \overset{\checkmark}{K_{cR}}(\overset{\checkmark}{x_{Dsp}} - \overset{\checkmark}{x_D}) \ldots$$

$$D = D_s + K_{cD}(m_{Dsp} - m_D)$$

$$V_B = V_{Bs} + K_{cV}(x_{Bsp} - x_B)$$

$$B = B_s + K_{cB}(m_{Bsp} - m_B)$$

CV	MV
x_D	R
✓ m_D	D ✓
x_B	V_B
m_B	B

sp = set point

Bias signal

So, degrees of freedom f equal to 4 N plus 11 minus 4 n plus 5 that is 6 that means this is under specified process, since V is greater than E. So, this is underspecified process, we need to make it exactly specified. So, what we need to do, we have to get f equal to 0, how we can get that there are 2 O S, we have discussed earlier, one is we need to specify more number of disturbance variables to reduce if to 0, we can specify more number of disturbance variables.

So, what are the disturbance variables involved in this distillation process, one is F, another one is Z. F is feed flow rate and Z is feed composition, we can maser this feed flow rate using a flow meter then, we have the feed flow rate information, we can maser this feed composition by any chromatography canalize. Then we have the confirmation information, if that is the case then F reduces to 4, previously F is 6, we are trying to specify this 2 disturbance variables that means, minus 2.

So, f becomes 4 what is the another option to make the process exactly specified, we can incorporate more number of control equations. So, second option is we can incorporate more number of controller equations. So, before writing the controller equations, we need to couple controlled variable, manipulated variable pears, what are the control variable and manipulated variable pears to be consider, for the example column, that we need to decide. So, control variable, manipulated variable see this is a distillation example feed is introduced on a particular tray, we are getting 2 products, one is the top product, another one is the bottom product.

So, what is the control object see for this process, control objective is to mention the composition products purity that means, we can consider one control variable as top product purity, which is represented by top product composition. Another controlled variable, we can consider that is the bottom product composition x B. Now what will be the manipulated variable for x D, we can consider the manipulated variable that is reflux flow rate and for bottom purity, we can consider the manipulated variable as vapor boil operate.

These are the standard control variable, manipulated variable pears along with this 2 pears, we can include another 2 control variable, manipulated variable pear. One for top section and one for bottom section, you see the reflux drum holdup is represented by m D, basically in the reflux drums some liquid is accumulated and that we represent by m

D. So, we can control that liquid height and that liquid height, we can control by the adjustment of distillate flow rate some liquid is accumulated after condensation in the reflux drum.

So, there is a scope to maintain the liquid holdup or we can say there is a need to maintain the liquid holdup in the reflux drum. So, if that is our objective, we can consider m D as the control variable and that can be adjusted by the outlet flow rate D by the similar fashion, we can consider the holdup in the in the column base m B as a another control variable.

Some liquid is accumulated in the column base, which is represented by m B. If that is our objective I mean, if we one to maintain the liquid holdup in the column base then that is the control variable and this m B can be manipulated sorry, this m B can be controlled by the manipulation of outlet liquid flow rate that is B.

So, these 4 controls manipulated control variable pears, we can consider for the example column. So, one manipulated variable is R and the controller equation although did not discuss that particular discuss later, I am just adding, I am just writing the equations controller equations. If R is the manipulated variable then one controller equation is R S plus K C R x D S P minus x D. Previously, we have used suffix D for the desired value here, we are using S P, S P is a set point. S P means, S P denotes set point.

Set point is nothing, but the desired value and this R S is a steadiest value of R in process control, we call R S as bias signal, that is basically the steadiest value of reflux rate R. K C R is the controller parameter, which we need to determine or we calling tuning parameter that is basically, constant term x D S P is the x D set point that means, that is the desired value of x D and this is a actual x D.

So, this is one equation similarly, we can write for D, D S plus K C D m D set point minus m D. For V B, we can write V B equals to V B S plus K C V x B set point minus x B and last equation is B equals to B S plus K C B m D set point minus m B. These are the control equations total 4 equations.

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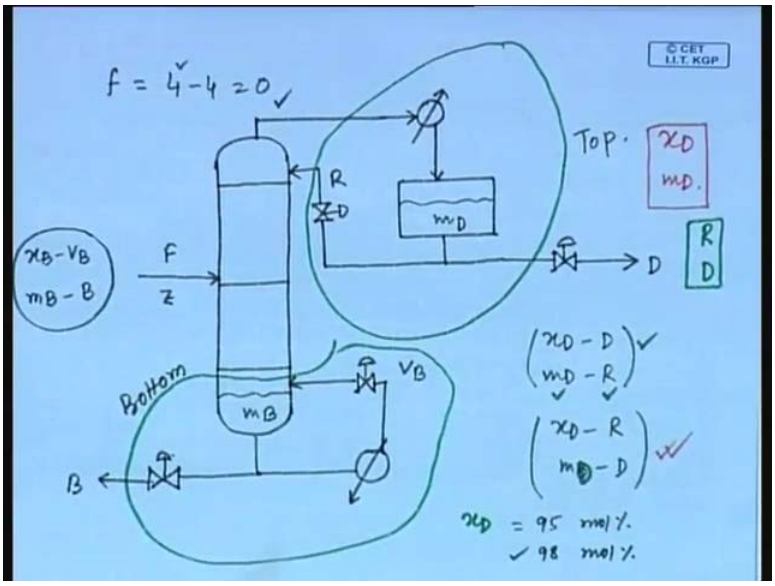

So, if we include 4 equations then degrees of freedom becomes 0, previously we had degrees of freedom equal to 4 after defining 4 control equations, our degrees of freedom becomes 0. Now, you will discuss how we can select the manipulated control variable pear for the example system, how we have selected this 4 control variable manipulated variable pears.

That will discuss in brief, this is the distillation tower feed flow rate with composition, one condenser is installed that the top, this is the reflux drum, liquid is accumulated here, the holdup is m D, this is the top stage. Suppose, this is a control wall, which is use to manipulate the reflux rate, this is another control wall, which use to manipulate distillate flow rate, this is reflux flow rate. At the bottom section, this is say bottom tray, this is feed tray some amount of liquid is accumulated here.

Now, this is the reboiler, this is one control wall, which is use to manipulate vapor boil operate, another outlet section is included for the out flow of bottom flow rate. Now will consider first the top section, I mean this section, this is the top section, in this top section, you see we have selected 2 control variable based of our control objective, one control variable is x D, another control variable is m D. This 2, we have selected based on our control objective.

So, how many equations are available for manipulation in the top section, 2 equations, 2 variables are available for manipulation, what are those variables, one is R another one is

D, this 2 variables are available for manipulation. Now, we have to pear the control variable and manipulated variable, we can pear x D D and m D R another pear may be x D R and m B D.

So, these are 2 possible pears first we will consider the first pear, we want to manipulate suppose m D, we want to control m D by the manipulation of R that is no problem, we can do that. If we consider the control of m D by the manipulation of R, we can easily do that there is no problem, because this is also outflow, I mean this is also outlet flow, this is also outlet. So, we can choose any one for controlling the m D.

Another option is x D verses D, suppose we have the distillate composition at present time 90 percent, I mean the distillate purity presently is 95 mole percent. Now I we want to change it to 98 mole percent purity, it is perhaps not possible to get 98 mole percent purity by the manipulation of distillate. But, it may be possible to get 98 mole percent purity by the manipulation of reflux flow rate.

Because, if we want to get 98 mole percent purity, there is a need to increase the reflux flow rate, which will affect the separation in the process and they are may be improvement of composition in the top section. If we want to increase x D, there is a need to infuse reflux flow rate, that will affect the separation in the process and then there may be some improvement in composition.

It is usual for binary distillation column, if we want to infuse x D, there is a need to infuse reflux flow rate, because we are not allowing to live the process, we are again treating that steam in the process. So, that there is some improvement can be achieved.

So, x D verses D is not a good option and the second option gets preference, I mean x D verses R and this is not m B, this is m D, m D verses D, this is best option among this 2. But, the similar O F or the bottom section is this one, this one is the bottom section by the similar o a for the bottom section, we chose x B verses V B and m B verses B, you see m B can affect the can affect the process, but B is leaving the process.

So, by the similar way as we discuss for the top section, this is the best option for the bottom section x D verses V B and m D verses B, this is all about the mathematical modeling degrees of freedom analyzes of a distillation column. Next, we will start I mean, we will just try to know in brief the Laplace transform, I hope you have started this in your basic mathematics course. So, we will not discuss in detail, but will recall the Laplace transform by some standard formulas.

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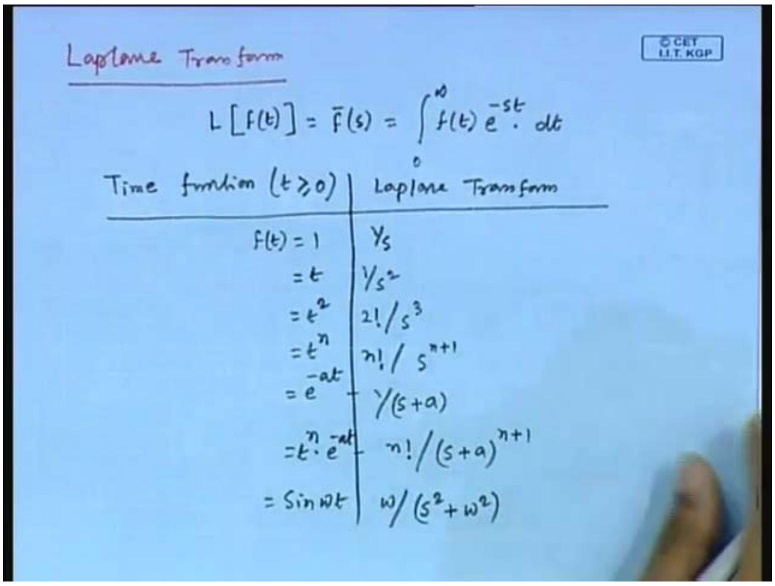

Laplace Transform

$$L[f(t)] = \bar{f}(s) = \int_0^\infty f(t)\, e^{-st} \cdot dt$$

Time function $(t \geq 0)$	Laplace Transform
$f(t) = 1$	$1/s$
$= t$	$1/s^2$
$= t^2$	$2!/s^3$
$= t^n$	$n!/s^{n+1}$
$= e^{-at}$	$1/(s+a)$
$= t^n \cdot e^{-at}$	$n!/(s+a)^{n+1}$
$= \sin \omega t$	$\omega/(s^2+\omega^2)$

So, next we will start the Laplace transform and brief, we will know the standard formulas basic equation of the Laplace transform of a function f t, we represent by this, f is a function and t is a time independent variable. This is equal to f bar s the function, which is written in Laplace domain equal to 0 to infinity, function of t e to the power minus s t d t, this is the standard formula.

Now, we will just write the formula in terms of time function Hoyer time t is greater than or equals to 0 and the Laplace transform of those functions. If this function equal to 1, the Laplace transform is 1 by s function equal to t 1 by s squire, if this is equal to t squire factorial 2 by s cube.

If this function is t to the power n then this becomes factorial n divided by s to the power n plus 1, if this is e to the power minus a t Laplace transform of this 1 by s plus a this is 10 to the power n e to the power minus a t Laplace transform is factorial n divided by s plus a hole to the power n plus 1. If this is sin omega t omega divided by s squire plus omega squire.

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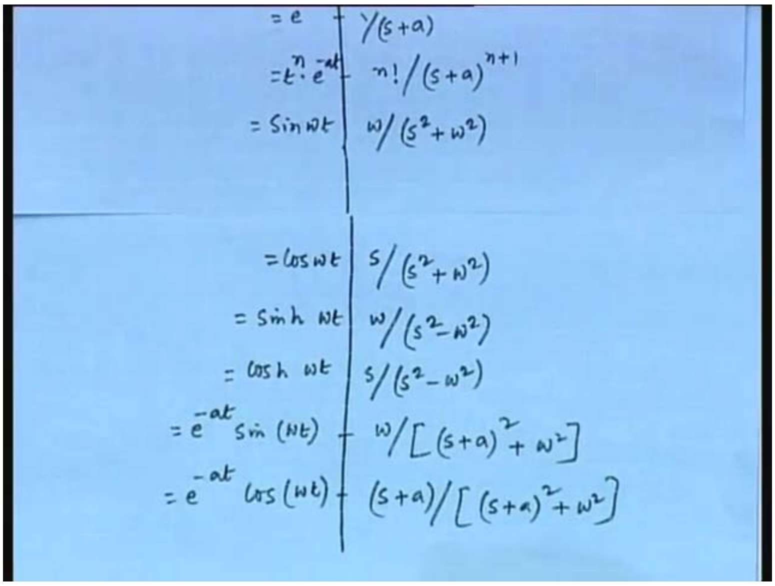

$= e$	$1/(s+a)$
$= t^n \cdot e^{-at}$	$n!/(s+a)^{n+1}$
$= \sin \omega t$	$\omega/(s^2+\omega^2)$
$= \cos \omega t$	$s/(s^2+\omega^2)$
$= \sinh \omega t$	$\omega/(s^2-\omega^2)$
$= \cosh \omega t$	$s/(s^2-\omega^2)$
$= e^{-at} \sin(\omega t)$	$\omega/[(s+a)^2+\omega^2]$
$= e^{-at} \cos(\omega t)$	$(s+a)/[(s+a)^2+\omega^2]$

Then this is equals to suppose, cos omega t s divided by s squire plus omega squre, this is sin hyperbolic omega t. Laplace transform is omega divided by s squire minus omega squire, if this is cos hyperbolic omega t, Laplace transform is s divided by s squire minus omega squire. Next one is exponential of minus a t sin omega t Laplace transform is omega divided by s plus a hole squire plus omega squire and e to the power minus a t cos omega t.

It has s plus a divided by s plus a hole squire plus omega squire, there are others functions are also define in different text books, I mean Laplace transform of different other functions more functions are available in text book. So, we will not discuss the Laplace transforms within a more functions.

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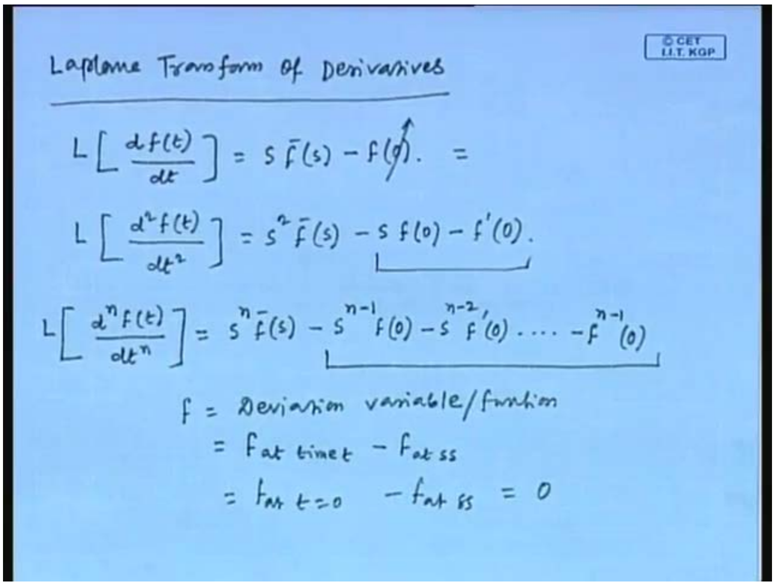

Laplace Transform of Derivatives

$$L\left[\frac{df(t)}{dt}\right] = s\bar{f}(s) - f(0). \quad =$$

$$L\left[\frac{d^2f(t)}{dt^2}\right] = s^2\bar{f}(s) \underbrace{- s\,f(0) - f'(0)}_{}.$$

$$L\left[\frac{d^nf(t)}{dt^n}\right] = s^n\bar{f}(s) \underbrace{- s^{n-1}f(0) - s^{n-2}f'(0) \ldots\ldots - f^{n-1}(0)}_{}$$

f = Deviation variable/function

$= f_{\text{at time } t} - f_{\text{at ss}}$

$= f_{\text{at } t=0} - f_{\text{at ss}} = 0$

So, we will next just consider the Laplace transform of derivatives, for the first order equation Laplace transform of d f t d t equal to s f bar s minus f naught. This is for first order differential equation, similarly if we consider second order equation d 2 f t d t squire, we get s squire f bar s minus s f naught minus first derivative of f naught. This is for the second order equation.

Similarly, for n third equation f t d t n equal to s to the power n f bar s minus s to the power n minus 1, f naught minus s to the power n minus 2, first derivative by this way last term will be n minus 1 derivative at 0. Now, if we consider f as the deviation variable, suppose f is a deviation variable means, f at any time t, the value of f at any time t minus the value of f at steady state, then we can call this variable f here, it is function as a deviation variable.

That means, if we consider this is a function. So, it is a function of deviation variables, if we consider f as a function f as a deviation function that means, it is a function of deviation variables. Now the definition of deviation variable is this, the variable at any time t minus the variable at steadies state. If that is the case I mean, if we consider, if as the function of deviation variables, what will be this first derivative, I mean the Laplace transform of first derivative, this will become 0 is not it.

That means, in this t equals to 0. So, f at t equals to 0 minus f steady state, we usually consider time t equals to 0 is steady stage. So, this becomes 0, similarly this 2 term become 0, similarly all this terms equal to 0, it is a usual practices in process control the variables in the model are considered in the form of deviation variable.

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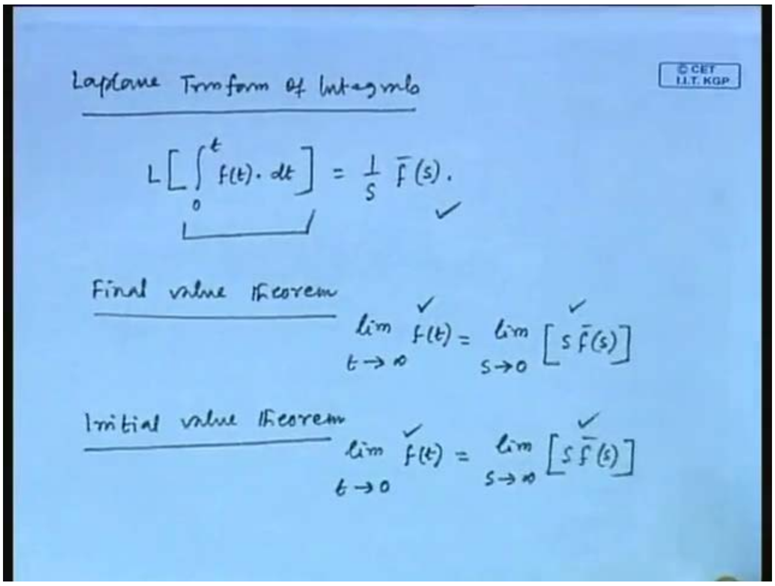

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Laplace Transform of Integrals

$$L\left[\underbrace{\int_0^t f(t)\cdot dt}\right] = \frac{1}{s}\bar{f}(s). \checkmark$$

Final value theorem

$$\lim_{t \to \infty} \overset{\checkmark}{f(t)} = \lim_{s \to 0} \overset{\checkmark}{\left[s\bar{f}(s)\right]}$$

Initial value theorem

$$\lim_{t \to 0} \overset{\checkmark}{f(t)} = \lim_{s \to \infty} \overset{\checkmark}{\left[s\bar{f}(s)\right]}$$

What is the Laplace transform of integrants, Laplace transform of integrals of function of t d t equal to 1 by s f bar s, if we consider f t as a function in time domain in the integration of that function is this one. And Laplace transform that function is this one by is f bar s, other 2 formulas are also used are also use in process control, those are final value theorem and initial value theorem. Final value theorem is limit t tens to infinity function of t equal to limit s tens to 0 s f bar s. This is the final value theorem, if our modeling equations are in time domain then, we have to consider this.

If our modeling equations are converted to Laplace domain in that case, we have to consider this. Another one is initial value theorem is limit t tens to 0 f t equals to limit s tens to infinity is f bar s. This is the initial value theorem, similarly if the modeling equations are in time domain, we have to consider this, if they are in Laplace domain, we can consider the right hand formula. So, these are about the in brief about the Laplace transforms. Next, we will go to discuss the different forcing functions, forcing function are usually the input variable.

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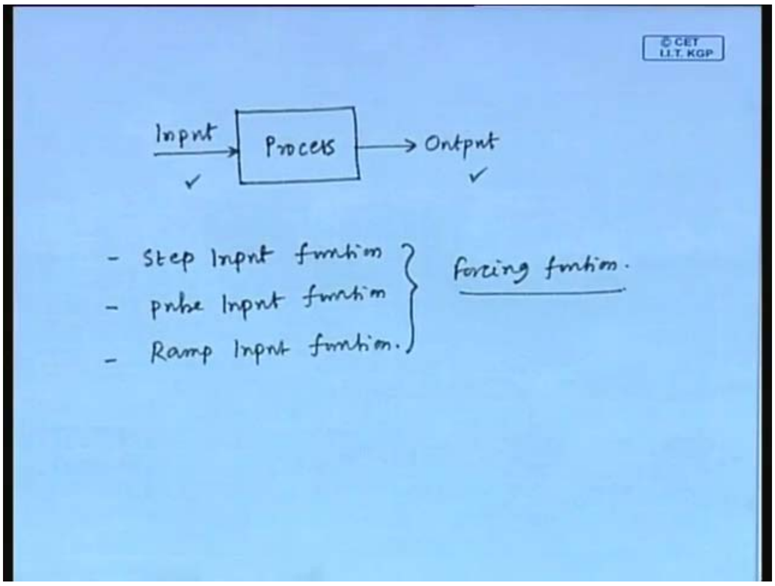

- Step Input function
- pulse Input function
- Ramp Input function.

} forcing function.

I mean, suppose we have a process, this is a chemical process, this is a input to the process and this is the output. Now, suppose initially the process is at steady state, we went to investigate the transient behavior of this process, we want to observe the dynamics of this process, how we can observe that by the use of simulator.

We have to introduce some change in input variable, if we give some change in input variable then, we will get some change in output variable that is basically, the transient behavior of a process or the dynamic characteristics of a process. So, what type of input variables, we will consider in our process control course. So, that corresponding output behavior, we can observe from the simulate that, we will discuss next.

Now, there are different input variables, which we will consider, those are like step input. Another one is pales input, it is better to write step input function, pales input function then ramp input function. So, these functions are basically called forcing function, I mean, we will use this name forcing function. Now, we will give change in input variable say by this fashion will give change in input variable as a step input then we will observe the output dynamics. Similarly, we can consider the pales chain in input variable then the effect in terms of output variable, change of input variable as ramp input, I mean ramp change then the transient behavior in terms of output variable that, we will discuss in the next class, fine.

Thank you.