# Mathematical Modelling and Simulation of Chemical Engineering Process
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## Lecture 38
## Simple Binary Batch Distillation

Hello everyone. Today we are going to talk about this Binary Batch Distillation. And then we will slowly see that how we can extend the idea of batch distillation to a more multi-component binary batch. So, before we talk about the batch system, it is very essential to understand that where batch systems or batch distillation is not something very common that we see.

So, batch distillation is generally useful when the product quantity is not too much. If it is a for example in pharmaceuticals, it is often we see or in very high specialty chemicals where it is very expensive and you cannot, you do not have a large volume or the large amount of the material to be processed then it is often preferred to have a batch system over a continuous system. Because continuous systems require a huge capital investment.

So, that is something we want to determine, I mean that is where the batch system is relevant. And also continuous systems are generally continuous. But if you know that there is an issue of the supply chain and you need the item has to be processed in batches and you have a storage tank and the quality of the raw materials differ from batch to batch to some extent, then batch distillation or any batch processing unit is preferred.

And this is particularly relevant for pharmaceutical stuffs or chemicals which have pharmaceutical applications because batch numbers or batches can have slight variations. So, that is why batch systems are relevant even though they do not operate in steady state and continuous system operating steady state but batch does not. But still batch systems are quite relevant and applicable in engineering context.

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## CONCEPTS COVERED

- ❖ Basics of batch distillation
- ❖ Constant reflux and constant distillate composition

Now, in this case of this binary batch system, first we will try to understand the basics of the batch distillation process. I mean taking an example of a binary system and then we will see what happens when you have reflux and constant distillate composition. How things change or what is the dynamics of the process.

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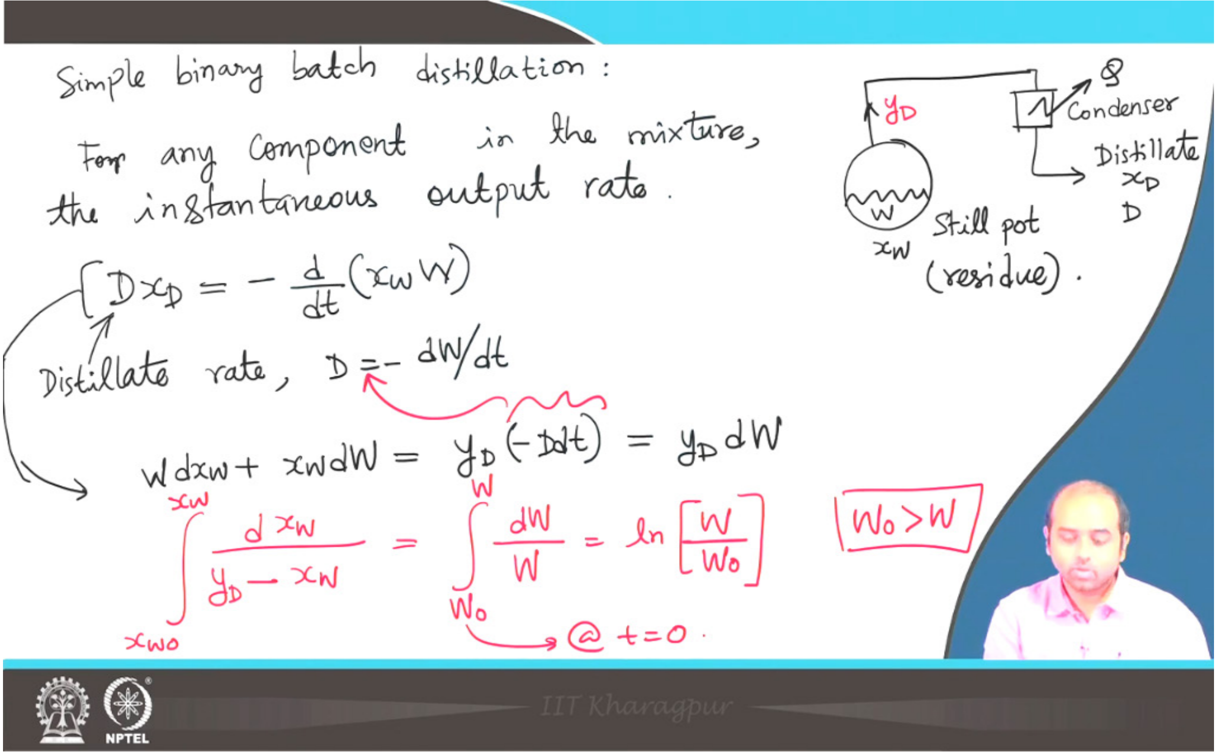

Simple binary batch distillation :

For any component in the mixture, the instantaneous output rate.

$$D x_D = -\frac{d}{dt}(x_W W)$$

Distillate rate, $D = -dW/dt$

$$W dx_W + x_W dW = y_D(-Ddt) = y_D dW$$

$$\int_{x_{W0}}^{x_W} \frac{dx_W}{y_D - x_W} = \int_{W_0}^{W} \frac{dW}{W} = \ln\left[\frac{W}{W_0}\right]$$

$W_0$ @ $t=0$.

$$\boxed{W_0 > W}$$

So, let us talk about a simple batch steel pot. Let us say this is a steel pot we are having. So, it is a steel pot. Let us say the steel pot has a volume W and the composition as x W. This is the residue. It is vaporizing. It is boiling. It is going up and here we are having a small, let us say condenser and we are getting the distillate. Distillate fraction is x D and the distillate rate is D.

So, please, note that W is the volumetric quantity in the steel part whereas D is the volumetric distillate rate taken out from the condenser. So, this is a simple batch, simple binary batch system we are talking about. So, for any component in the or let us say the more volatile component, the instantaneous distillate rate, instantaneous output rate or the distillate rate can be written down something like this.

So, this is the distillate rate of the, let us say, the higher volatile component or for any component, in fact, is minus the rate of change of the that product in the residue. This is nothing but the residue. So, this is a balance or this is nothing but I mean D is the instantaneous, I mean the D is the distillate rate. So, D is something we can write as minus d W by d t.

So, rate of change of the residue is equal to the amount that is produced in the distillate. That is what it is distillate rate and minus is means because with time W is decreasing. So, similarly, from the individual component mole balance we can also write that D of x D minus this quantity, I mean is the individual component mass rate or the volumetric rate, whatever you can say, is equal to minus D dt of this component.

So, this amount of residue or the volume still left in the steel pot. So, from here we get W, I mean doing the right hand side x W plus x W d W is equal to y D. x D is equal to y D, essentially. This is equal to y D d W. This is just algebraic steps we are representing left hand side, I mean this just expansion of x W W and x D I have written down as y D. Because y D is the vapor. So, this is y D.

Ultimately, when it is condensed, it becomes x D, that is a liquid phase composition. So, I can just do a integration of this stuff on the left and the right hand side, something like this. I can at least write the integral. So, it is W 0 is the initial W and at any time you will be getting W. Similarly, the initial x W is x W naught or any time t it is x W. So, this one will be ln W by W naught. So, W naught is always greater than W. So, W naught is the start at t is equal to zero. So, how do you evaluate the left hand side integral?

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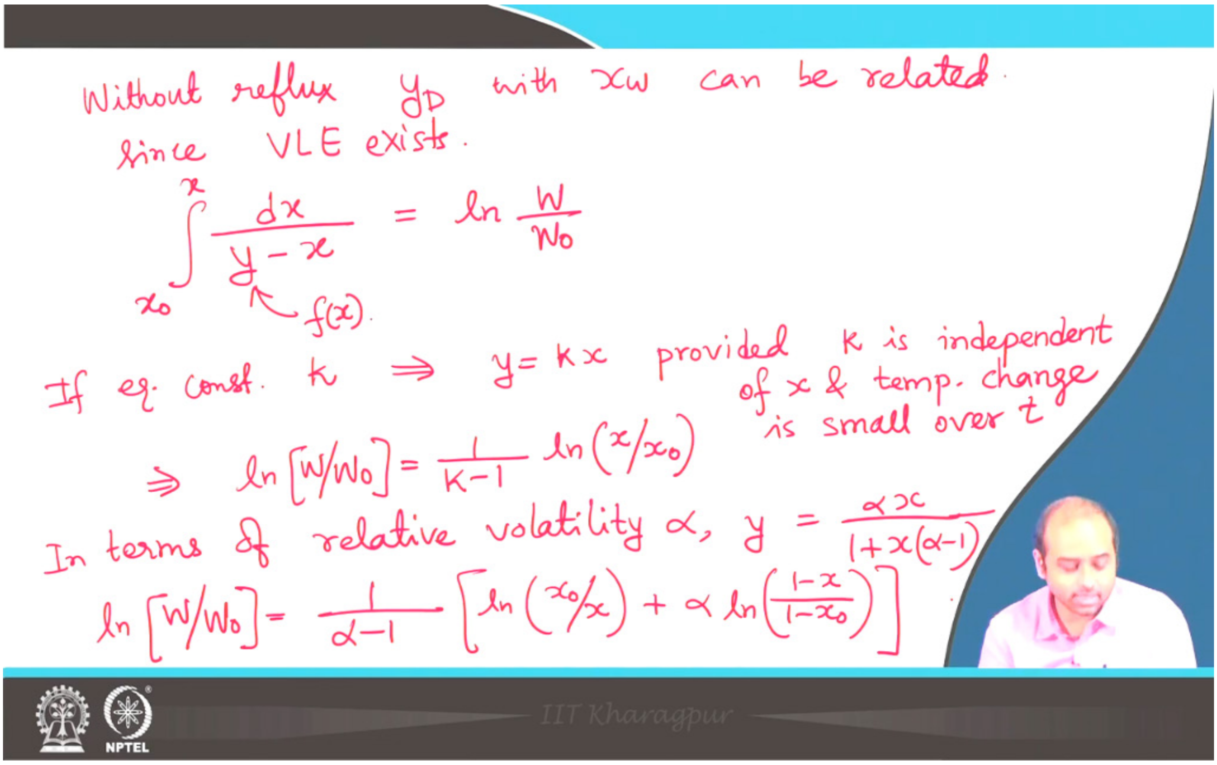

Without reflux $y_D$ with $x_W$ can be related.

since VLE exists.

$$\int_{x_0}^{x} \frac{dx}{y - x} = \ln \frac{W}{W_0}$$

$\nwarrow f(x)$.

If eq. const. k $\Rightarrow$ $y = kx$ provided k is independent of x & temp. change is small over t

$$\Rightarrow \ln\left[W/W_0\right] = \frac{1}{K-1}\ln\left(x/x_0\right)$$

In terms of relative volatility $\alpha$, $y = \frac{\alpha x}{1+x(\alpha-1)}$

$$\ln\left[W/W_0\right] = \frac{1}{\alpha-1}\left[\ln\left(x_0/x\right) + \alpha\ln\left(\frac{1-x}{1-x_0}\right)\right]$$

So, please note that without any reflux, we can relate y D with x W can be related, since they are in equilibrium, since really exist, vapor liquid equilibrium exist. So, in this integration, when you have d x by dropping the subscript notations x W by x is equal to ln W by W naught.

I can say that this is nothing but some function of x. So, if the K values, if the equilibrium constants K are known, I can always write that y is equal to K x provided K is independent of x which is generally the case. And temperature change is small over this time t that we are talking about, if that is small then I can write something that y is equal to K x.

And if this is the case then you can easily work out that the integration something like 1 by 1 minus K minus 1 ln x by x naught. And if you want to define in terms of the relative volatility which is also possible, in terms of relative volatility alpha where y is equal to alpha x by 1 plus x alpha minus 1. You know this for binary systems we can also always write this.

Then I will be getting ln something like this. So, all these cases are possible when you do not have reflux in the system. There is no reflux in the system. And in that case, this entire system can be considered as one single stage and W y is a direct function of x in one way or the other. Now, what happens when you have reflux in the system?

And let us say there could be two situations, one you have constant reflux and one where we want to set the product composition or the distillate fraction x D or y D to be not changing in time. So, constant distillate composition is something that we can set but the other one is that.

So, in that case, if you have reflux in the system then either you can have constant reflux. In that case the distillate composition will change. Or the other case where you want to have constant distillate composition in that scenario you have to change the reflux continuously to attain constant distillate composition.

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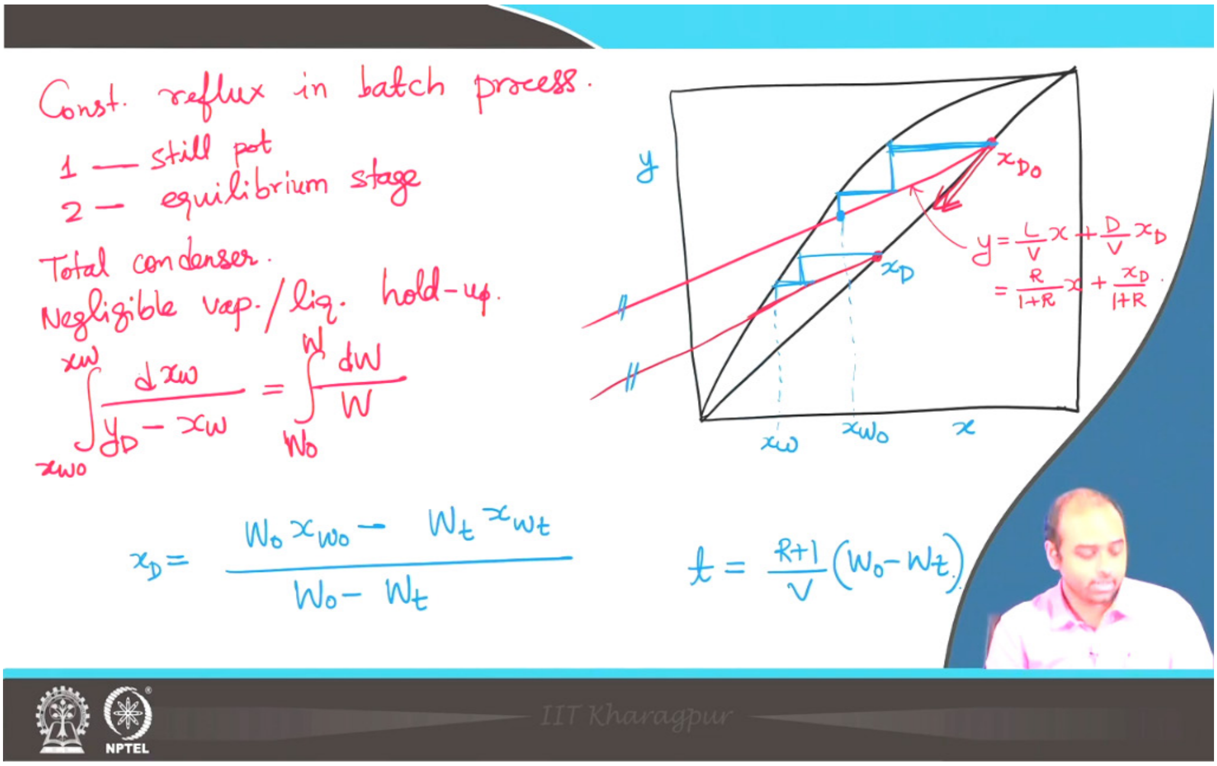

Const. reflux in batch process.

1 — still pot

2 — equilibrium stage

Total condenser.

Negligible vap./liq. hold-up.

$$\int_{x_{W0}}^{x_W} \frac{dx_W}{y_D - x_W} = \int_{W_0}^{W} \frac{dW}{W}$$

$$y = \frac{L}{V}x + \frac{D}{V}x_D = \frac{R}{1+R}x + \frac{x_D}{1+R}$$

$$x_D = \frac{W_0 x_{W0} - W_t x_{Wt}}{W_0 - W_t}$$

$$t = \frac{R+1}{V}(W_0 - W_t)$$

So, first look into the situation let us look into the situation of constant reflux in this batch process. So, let us consider I mean two stages, one is the steel pot. Let us say, another one is an equilibrium stage. So, you have a total condenser in the system and considering negligible vapor or liquid hold up.

So, the equation that we have here y and x W are not directly related. Because there is one more stage and you are having some reflux in the system. Now, let us try to have a graphical drawing here something like this. Let us say the initial point is x D 0 and I have a reflux like this. I mean that line operating line where the reflux needs to be known and what is the equation of the operating line. I think all of you are aware of this.

The equation of the operating line is y is equal to L by V x plus D by v x D. Or in other words I can write this as R by 1 plus R x plus R by R 1 plus R, this x D by R 1 plus R where R is the reflux ratio, all of you are aware of this. That is the equation. And to this equation I try to construct two stages. These will look something like this. So, two stage I am having here.

Now, what happens is that this is y and this is x we are having. So, this, I mean after drawings two stage whatever the value that you get here after the two stages, so, x D 0 is the top or the from the top whatever you are getting at the distillate. And the quantity here is what you are getting your x W. This is nothing but your x W.

So, now, when you are having, let us say, the R is constant and with time what will happen is that you are going to have decrease in the top product composition. So, x D will actually move along this line with time and at a future time it will again have a same reflux ratio. So, I can always draw a parallel line here.

And corresponding to the value of x W at that whatever the value of x W that I have, I can once again construct two stages. So, something like this I can construct and find out what would be my new x, this x D. So, this is a different x W and this would be like a new value of my x D.

So, with this graphical construction, as with time I can continue to, so, these are parallel lines. These are parallel lines because the reflux ratio is held constant. So, this has to be integrated numerically because y D has to be obtained from the graphical construction by drawing two equilibrium stages corresponding to the value of the x W, is just the reverse way around.

So, with x W, I try to draw two stages for that kind of slope that we are talking about and then try to see at what point this match or we get the value of our x W. So, that is something, this is how you can work out this integration, this with the help of numerical calculation. Because here, we cannot do the x, this y D and x W is not directly related, it is not a single stage calculation, they are not directly related.

So, they can only be related with the multi-stage calculation by doing this graphical construct. So, from here, you can just from the mass balance, you can find out that this x D can be related in sort of this way. This is from the mass balance we can always write it down that whatever loss of the quantity that we had for this component or the volatile component in the residue is actually gained in the top distillate depending on how much of the amount that is lost.

This is something we can always work it out and this is the way to calculate out what would be your x D, in the same way how we calculate out what would be in the previous case, what would be your x D, provided it is a single stage calculation. And you can also find that the time required for this process can be written down in this way.

Again from the balance of the residues. I am talking about the reflux ratios. So, now, let us look into the situation of the constant distillate composition. So, the constant distillate composition, we can write down I mean we can write down.

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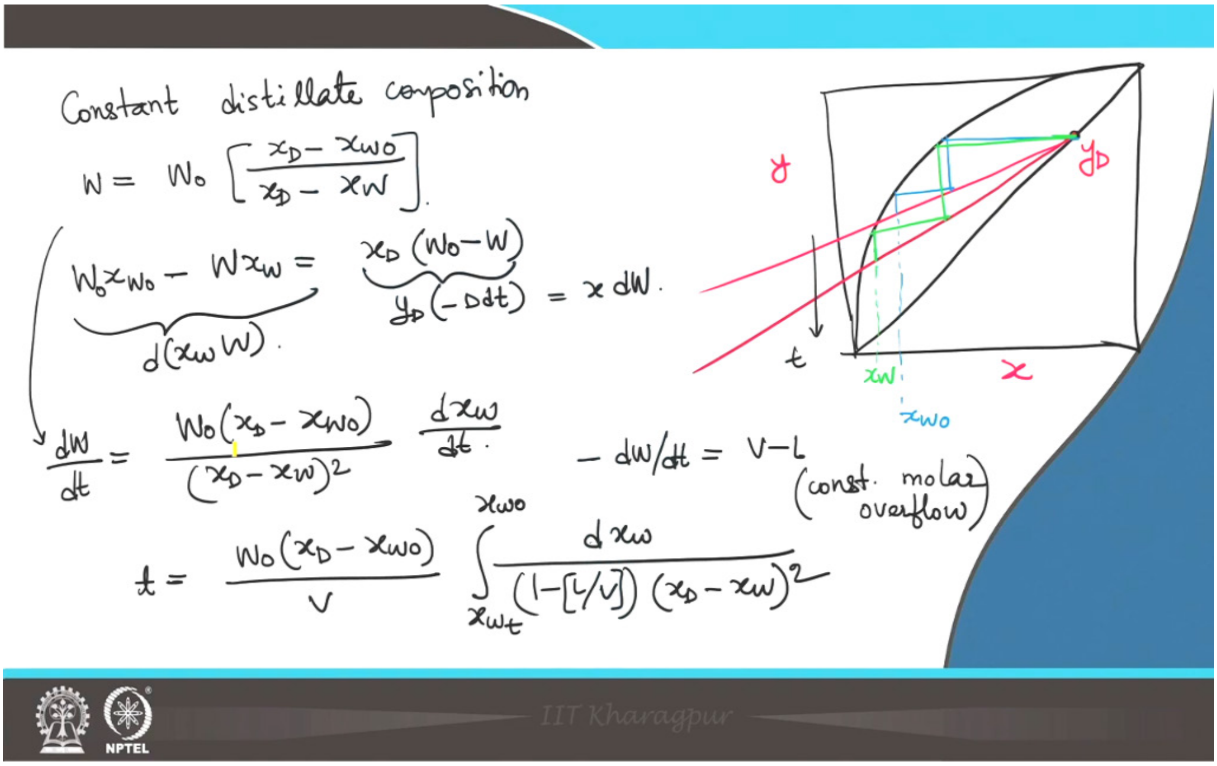


Constant distillate composition

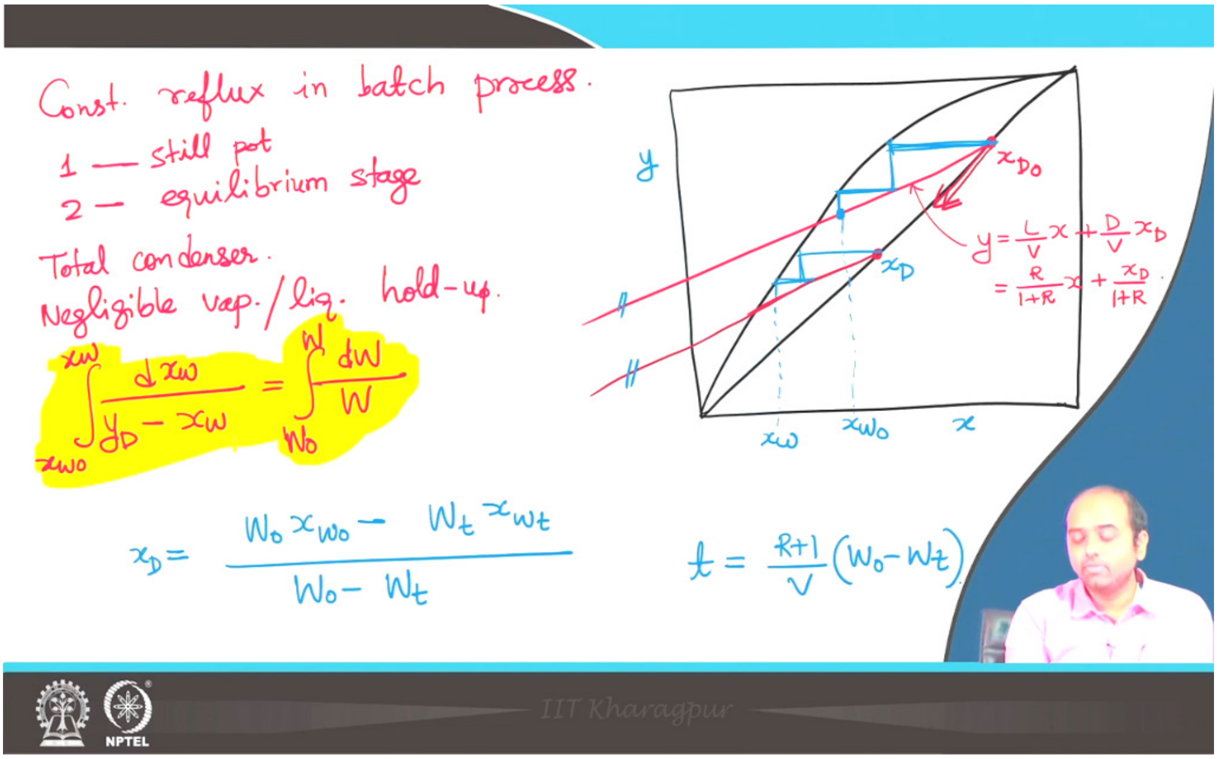
$$W = W_0 \left[ \frac{x_D - x_{W0}}{x_D - x_W} \right].$$

$$\underbrace{W_0 x_{W0} - W x_W}_{d(x_W W)} = \underbrace{x_D (W_0 - W)}_{y_D(-D\,dt)} = x\,dW.$$

$$\frac{dW}{dt} = \frac{W_0 (x_D - x_{W0})}{(x_D - x_W)^2} \frac{dx_W}{dt}. \qquad -dW/dt = V - L$$

(const. molar overflow)

$$t = \frac{W_0 (x_D - x_{W0})}{V} \int_{x_{Wt}}^{x_{W0}} \frac{dx_W}{(1 - [L/V])(x_D - x_W)^2}$$



Const. reflux in batch process.

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$$\int_{x_{W0}}^{x_W} \frac{dx_W}{y_D - x_W} = \int_{W_0}^{W} \frac{dW}{W}$$

$$x_D = \frac{W_0 x_{W0} - W_t x_{Wt}}{W_0 - W_t}$$

$$t = \frac{R+1}{V}(W_0 - W_t)$$

$$y = \frac{L}{V}x + \frac{D}{V}x_D = \frac{R}{1+R}x + \frac{x_D}{1+R}$$

Let us try to work the graphical method once again. So, the only way to obtain constant distillate composition is by altering the reflux ratio. This is also true for continuous systems. The only way to obtain constant distillate composition is by altering the reflux ratio. How? So, let us say this is our y D. So, this is y versus x curve.

So, initially, let us say with a certain amount of reflux ratio, we are getting this equation, I mean this line. And here somehow, I am able to, the drawing is not good but let us say, somehow, I am able to construct two stages. No, I cannot draw like that. I should not draw like this. This second draw, two stage like this.

Let us say this is the scenario at the beginning when we had x W 0. Now, with time, if you want to maintain the same x y D and to find out that how x W changes, the only way that you can achieve is by altering the reflux ratio. So, for a different case, where I can have that same amount of x D, so, I can draw a curve like this.

And again here try to construct the two stages maybe in a different color something like this. This is possible. So, we see that with time, the reflux ratio is changing. So, these lines are not no longer parallel and the change of the slope of these lines suggests that the reflux ratio is changing. So, for constant, I mean distillate composition, the only way that you can achieve is that by altering the reflux ratios.

So, in this case you have, I can work out to some extent. I mean the same equation still holds and I can write down something like this. This always holds, from the mass balance you know that we have x W 0 minus W x W is equal to x D W 0 minus W.

Because this part is nothing but y D minus D delta t, if you recall. And this is equal to nothing but x into d W. So, this part is d of x W W. This always holds. So, d W d t, from here I can work out as W 0 x D minus x W 0 by x D minus x W square d of x W by d t. And you also know that d W by d t minus d W by d t; you can say something like constant molar overflow or something like that.

The distillate rate can be given by the loss of the W. So, the time that you can work out, if you do the integration and you can write down something like this, this will tell you the time required for this distillation to attain x W starting from a concentration of x W naught. So, this is for constant molar overflow, based on the same assumptions the McCabe-Thiele theory method is also valid. So, this we can use and to calculate the value of L by V.

And you can find out that from the numerical integration you can calculate out that how changing your R will change your W. So, again you are going to once again use the same equation. So, this is the same equation that you will be using here in this case 2. But you know that how y D is related to x W, when you have constant reflux and when you have constant distillate composition.

In the top where y D would be fixed but how x W is changing, that is something you can work out for this case of two stage. I believe that you get a good glimpse of the idea of this batch distillation, where there could be two possible scenarios. I mean batch also could have stages, equilibrium stages.

And you can have two scenarios, one in the case of the constant reflux and another is the constant distillate composition. And you can see that how in those two cases, the composition in the residue is related to the top distillate composition. And once you know that relation, you can work out the integration and then you can find out that how x W is changing with respect to time. That is the objective and that is something we wish to calculate in this process of the batch. Thank you.

So, this is, please, note that this is a transient phenomenon. So, things are changing with respect to time. So, we are interested to work out how does the residue composition change with time. How does this residue volume or the mass also change with respect to time. Thank you and then in the next class we are going to talk about this multi-stage multi-component batch distillation and how we can write the similar type of the mesh equations in that context. Thank you. I hope all of you like this lecture in this class.