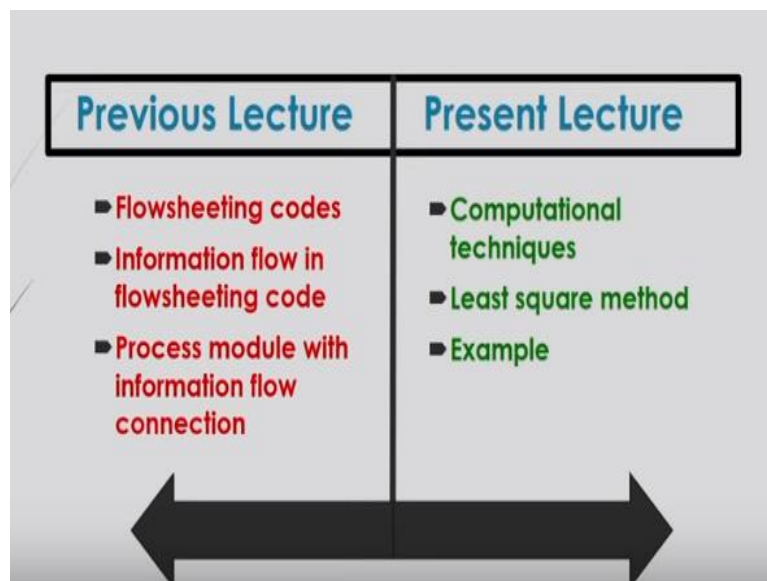


**Basic Principles and Calculations in Chemical Engineering**  
**Prof. S. K. Majumder**  
**Chemical Engineering Department**  
**Indian Institute of Technology-Guwahati**

**Lecture - 29**  
**Least Square Method Linear Equation Fitting**

Welcome to massive open online course on Basic Principles and Calculations in Chemical Engineering. Today we will start module 10, which is about the computational techniques and in this lecture we will try to discuss about the least square method by which how to fit the linear equation graphically based on the experimental data.

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And for that we have actually discussed that how to fit that or how to make a differential equation or you can how to make the energy balance equation, material balance equation based on the chemical process and to solve those you know material balance equation or energy balance equation, whether it is linear or nonlinear, you need to solve those equations.

Now there are several, you know way to solve those equations. Basically, to solve those equations either you can do numerically or by you know that analytically. Now to solve that analytically, you know that you have to you know manage those equations, either by multiplying or dividing the coefficients and eliminating some coefficients from one equations and comparing to other equations.

After that either subtraction or addition, you will see that you can eliminate some variables and those variables after that, you can you know get just by you know solving, if it is coming one single equation based on which you can solve that single variable from those equation.

You will see that since there are you know various chemical engineering operations where you need to sometime you know predict that dependent variables like you know that suppose, any fluid is flowing through the pipe then there you will see that there will be a frictional pressure drop will be changing based on the you know that variables like velocity like diameter of the pipe.

Even you can say that fluid proprieties. Now you need to sometimes predict those you know a change of pressure drop based on that variables just by you know just proposing an equation. Whether it may be linear or nonlinear that will be you know based on that you know experimental data on that particular you know results, in this case like fictional pressure drop.

Like other also you can say that like suppose you want to you know predict some output of the process like process efficiency or yield or you can say that suppose heat transfer coefficient, mass transfer coefficient, those you know variables are called the dependent variables, why? Because these variables depends on different operating variables.

Now in that case, suppose heat transfer coefficient will be depending on the you know Reynolds number and how that dispersion coefficient will be you know changing with the Reynolds number, even other variables that also can be predict based on the experimental data.

Now to you know make that one you know empirical equation or any you know that linear equation based on that experimental data you need to sometimes you know estimate the coefficient of that equation based on which you can say that this equation will be you know predicting that experimental data.

Now in generally if we consider that, that dependent variables will be you know a function of some independent variables like in case of suppose fluid is flowing through the pipe, their frictional pressure drop will be you know varying with that you know fluid properties like viscosity, density, even surface tension and also pipe diameter and also you can say that velocity of the fluid.

So this velocity, pipe diameter, viscosity, density, surface tension those are independent variables based on which you can say that, that pressure drop, friction of pressure drop which is dependent variables will be changing.

Now let us consider that how to actually fit that frictional pressure drop or suppose any in general dependent variables depending on that independent variables, how one can you know develop an equation and how that equation can be fitted with that experimental data. For that you know dependent variables based on that independent variables.

Now to find out those you know or make that equations you need to solve that equation coefficient either by least square method or numerically based on other you know computational programming method. Now let us consider that least square method here by which you can you know develop an equation to predict that experimental data.

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**Method of least square**

- Sometime we need to express experimental results of any depended variable by an equation
- For that you need to estimate the best values of the coefficients in the equation from experimental data. The equation might be a theoretical law or just a polynomial, but the procedure is the same.
- Let  $y$  be the dependent variable in the equation,  $b_i$  be the coefficients in the equation, and  $x_i$  be the independent variables in the equation so that the model is of the form

$$y = f(b_0, b_1, \dots; x_0, x_1, \dots)$$

e.g.  $y = b_0 + b_1x$

Now what is that you know least square method? Sometimes we need to express that experimental results of any dependent variable by an equation. Now let us consider that equation which will be you know expressing by dependent variables and independent variables.

Let us consider that dependent variables as  $y$  and independent variables are  $x_0, x_1$  like this. Now if we propose an equation based on this dependent variable and independent variables like then  $y$  is equal to  $b_0 + b_1x$ . Now here this is an equation, which is only one variable here  $x$ , whereas this  $b_0$  and  $b_1$  these are coefficients.

And these coefficients you know can be you know estimated if you fit this equation with the experimental data. But whenever you will be fitting these experimental data with this equation you will have some error, because your this equation will not give you that 100 percent correct data of that experimental data.

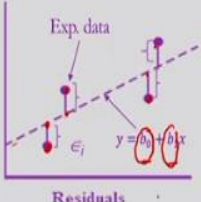
Or you can say that there will be a sudden deviation of this you know predicted equation or proposing equation based on that experimental data from that experimental results. Now how to estimate this  $b_0$  and  $b_1$  coefficients and what will be the goodness of feat of this equation with that experimental data you need to know.

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■ Let  $\epsilon$  represent the error between the **experimental value,  $Y$** , and the predicted value of  $y$  using the values of  $x_i$  and the estimated values of the coefficients  $b_i$ :

$$\hat{Y} - y = \epsilon$$

■ The best way of estimation of the coefficients is by least squares, that is, by minimizing the sum of the squares of the errors (of the deviations) between  $Y$  and  $y$  for all the  $i$  sets of experimental data:



$$\text{Minimize } F = \sum_{i=1}^n (\epsilon_i)^2 = \sum_{i=1}^n (Y_i - f_i)^2$$

Now let us find out these things here in this lecture, suppose that if epsilon the error between the experimental value and you know that propose you know equation. So

this experimental value is capital Y and this y dependent variables will be obtained based on that equation  $y$  is equal to  $b_0$  plus  $b_1 x$ .

Now error between these two you know values is representing by you know epsilon. Now this epsilon of course, there will be a certain error between this. This is deviation or epsilon you can see in this figure here. This is your experimental data. These are your experiment data and this dotted line is representing that data which can be obtained by that equation  $y = b_0 + b_1 x$ .

Now if you consider this experimental data, and the data obtained by this equation here, there will be a certain error. So this error is represented by epsilon. Similarly, for other points also there will be an error. Similarly, here also there will be another error. Here also there will be another error.

But all those error, if you consider individual data of that experiment and individual data obtained by that equation, they may not be same. There may be you know that some small error maybe bigger error maybe even that all the values of this error will not be uniform in value or you know that number.

So in that case, you know that you have to optimize this error so that you can get that less percentage of you know deviation of this experimental this proposed equation. So you have to optimize this you know error there. And based on that optimization in this case you have to minimize this error.

So the best way of estimation of the coefficients, here  $b_0$  and  $b_1$  can be obtained if you minimize this error there. Now by minimizing the sum of the squares of the error or between these  $y$ 's, capital Y and small  $y$  for all the  $i$  set of experimental data, you can write here minimize of this  $f$  function.

That will be is equal to here basically that  $\epsilon_i$  whole square and this is for  $i$ th component. So for all components you have to sum it up. So summation of all square of these errors if you can minimize then you can get that you know best value of this  $b_1$  and  $b_0$  from the experimental data.

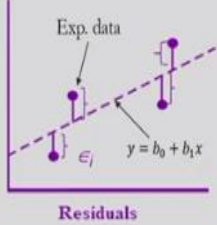
So that you can get least error so that you can get less percentage error of this experimental data with the proposed equation. So here let it be considering here this epsilon i which is to be minimized. Now this epsilon i is basically  $Y_i - f_i$ . What is this  $f_i$ ,  $f_i$  is basically a function that we have considered here,  $y = b_0 + b_1x$ . So this equation to be minimized here.

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- Consider a model linear in the coefficients with one independent variable  $x$

$$y = b_0 + b_1x$$

- The objective function is

$$F = \sum_{i=1}^n (Y_i - y_i)^2 = \sum_{i=1}^n (Y_i - b_0 - b_1x_i)^2$$


- There are two unknown coefficients,  $b_0$  and  $b_1$ , and  $p$  known pairs of experimental values of  $Y_j$  and  $x_j$ .
- You have to minimize  $F$  with respect to  $b_0$  and  $b_1$ .

Now consider that model linear equation in the coefficients with one independent variable  $x$  that is  $y = b_0 + b_1x$  as a function there. So here the objective function will be is equal to here that  $F$  will be is equal to summation of  $i$  to  $n$   $Y_i - Y_i$  whole square. That will be is equal to here simply  $Y_i$  means here, this one this function.

So  $Y_i - b_0 - b_1x_i$  whole square. Here in this case, we are getting two unknown coefficients. There may be more than one and more than two unknown coefficients. There also you have to do in this way, what should be the error which is to be minimized. Now there are two unknown coefficient in this case  $b_0$  and  $b_1$ .

And also we can have that there will be a certain pairs of experimental values of  $Y_j$  and  $x_j$ . Here you have to minimize this  $F$  with respect to that  $b_0$  and  $b_1$  there.

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- The necessary conditions for a minimum error:
 
$$\frac{\partial F}{\partial b_0} = -2 \sum_{i=1}^n (Y_i - b_0 - b_1 x_i) = 0$$

$$\frac{\partial F}{\partial b_1} = -2 \sum_{i=1}^n [Y_i - b_0 - b_1 x_i] x_i = 0$$
- Rearrangement yields a set of linear equations in two unknowns,  $b_0$  and  $b_1$ :
 
$$\sum_{i=1}^n b_0 + \sum_{i=1}^n b_1 x_i = \sum_{i=1}^n Y_i$$

$$\sum_{i=1}^n b_0 x_i + \sum_{i=1}^n b_1 x_i^2 = \sum_{i=1}^n x_i Y_i$$

Now if we apply that necessary conditions for a minimum error, that means here doh F doh b 0. That should be is equal to zero because to minimize that this differentiation will be equals to zero as per necessary conditions. So we can express this equation here -2 ino summation of i is equal to 1 n Y i – b 0 – b 1x i.

Similarly, that error with respect to coefficient b 1that can be expressed like this. Now for minimum error, this will be equals to zero and this will be equals to zero. Now rearrangement of these two equations, we can write a set of linear equations in two unknowns, here b 0 and b 1. So we can write here from these two equations here, summation or b 0 plus summation of b 1x i. That will be is equal to summation of Y i.

Similarly from this equation 2 here, let it be this equation, this equation 1 and this equation 2. So from these two equations, you can write this two linear equations as a sum of that square of that variables and also here product of that x i and Y i. So from these two equations, we can solve for b 0 and b 1 just by elimination techniques or either way or other methods.

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$$nb_0 + b_1 \sum_{i=1}^n x_i = \sum_{i=1}^n Y_i \quad \checkmark$$

$$b_0 \sum_{i=1}^n x_i + b_1 \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i Y_i \quad \checkmark$$

The two linear equations above in two unknowns,  $b_0$  and  $b_1$ , can be solved quite easily for

$b_0$  = intercept and  
 $b_1$  = the slope.

Now from those equations we can write after simplification or rearrangement like this in this way this and this. Now the two linear equations here above as shown here in the slides, here two unknown so two linear equations we are getting. So we can solve this equation and we can get the solution for you know  $b_0$  and  $b_1$ .

And now this  $b_0$  and  $b_1$  coefficient is basically intercept and the slope, if you are considering that equation as a straight line equation, so in that case  $b_0$  will be intercept and  $b_1$  will be is equal to slope.

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$$b_0 = \frac{\sum Y_i \sum x_i^2 - \sum x_i \sum x_i Y_i}{np \sum x_i^2 - (\sum x_i)^2}$$

$$b_1 = \frac{p \sum x_i Y_i - \sum x_i \sum Y_i}{np \sum x_i^2 - (\sum x_i)^2}$$

So, the model equation will be

$$y = b_0 + b_1 x$$

Now after solving these two linear equations, we can express the coefficients in terms of that independent and dependent variables here by this here. So we can write here  $b_0$  is equal to here this based on this equation. Here  $p$  is this number of datas or you



can write here n also instead of p here n. So it will be n number of data n also you can write.

So b 0 can be calculated by this equation and b 1 can be calculated by this equation. So the model equation will be is equal to  $y = b_0 + b_1x$ . Now this b 0 and b 1 will be you know calculated based on this you know equation, which is basically as a function of that experimental data of that variables.

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**Goodness of fit**

**Sum squares**

$$SS_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2$$

$$SS_{yy} = \sum_{i=1}^n (Y_i - \bar{Y})^2$$

$$SS_{xy} = \sum_{i=1}^n (x_i - \bar{x})(Y_i - \bar{Y})$$

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \quad \bar{Y} = \frac{1}{n} \sum_{i=1}^n Y_i$$

**Correlation Coefficient,**

$0 < R^2 < 1$

$R^2$  value tends to 1 reflects the better fit of the model

$$R^2 = \frac{SS_{xy}^2}{SS_{xx}SS_{yy}}$$

$$SE(b_0) = s \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{SS_{xx}}}$$

$$SE(b_1) = \frac{s}{\sqrt{SS_{xx}}}$$

$$s = \sqrt{\frac{SS_{yy} - \frac{SS_{xy}^2}{SS_{xx}}}{n - 2}}$$

Now how you know good this you know equation to be fitted with the experimental data with list error that you have to assess there. Now to access this equation, you have to find out one coefficient that is called correlation coefficient. This correlation coefficient is significant because this will give you that how or what extent of goodness or fitness of that equation with the experimental data.

So this is basically represented by the notation R square. So this R square is called correlation coefficient. This is defined as by this equation here. Now this R square value if it is coming near about to 1, not greater than 1, then you can say that the equation will be well fitted with the experimental data.

But if it is coming below, you know 0.90 we will see that there will be a huge deficient of the experimental data with the data given by this equation. So in that case you have to find out that goodness of fit of that equation. If your equation is not

giving that R square value near about 1 you cannot propose that equation to predict the experimental data.

Now how to find out this correlation coefficient. Now to find out this correlation coefficient, you need to you know sum squares of you know variables there. Now what is that sum square of variables here? We will see we have defined here you have given here in this slide some equations for that.

You have to calculate first this  $SS_{xx}$ . What is this sum squares for x values, that is independent values. What is that? This is basically defined as summation of  $x_i$  minus  $\bar{x}$  whole square. What is the  $x_i$ ?  $x_i$  is the independent variables or  $\bar{x}$  is the average of that independent variables.

That average of that independent variables can be calculated based on this equation here simply you have to sum it up that independent variables and divide it by number of here data. So you can obtain this  $\bar{x}$  here. Similarly,  $SS_{yy}$  you can calculate based on this equation which is defined as summation of  $Y_i$  minus  $\bar{Y}$  whole square.

Here  $Y_i$  is the you know dependent variables whereas  $\bar{Y}$  is the average value of that dependent variables based on that experimental data and then  $SS_{xy}$  is basically that  $x_i$  minus  $\bar{x}$  into  $Y_i$  minus  $\bar{Y}$  and then you have to sum all those data. So product of this deviation of  $x_i$  from mean and deviation of  $Y_i$  from its mean and then sum.

So it is called  $SS_{xy}$ . It is called sum squares of x y. Now after that if you get this value up  $SS_{xx}$ ,  $SS_{yy}$  and  $SS_{xy}$ , you just substitute that value here in this equation, you can get this R square value. Now you will see there will be a sum standard error of this you know  $b_0$  coefficient and  $B_1$  coefficient here.

So that standard error or that  $b_0$  based on that  $b_0$  you can obtain based on this sum square and this average value of dependent variables and also how many numbers of experimental data is there. So in this case it is defined as like this  $S$  into root over  $1$  by  $n$  plus  $\bar{x}$  square divided by  $SS_{xx}$ .

So from this equation, you can obtain what will be the standard error or B 0. And similarly standard error for b 1 it will be S by root over SS xx. Whereas S is defined as this root over SS yy minus SS xy square divided by SS xx divided by n - 2. Here n is the number of experimental data.

So in this way you can find out if you propose any equation to predict your experimental data, how or what extent of goodness of fit that you know experimental data with your proposed equation.

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**Example**

$x:$  1 2 3 4 5  
 $y:$  2.5 3.5 5 6.5 7

$b_0 = \frac{\sum y_i \sum x_i^2 - \sum x_i \sum x_i y_i}{n(\sum x_i^2) - (\sum x_i)^2}$ ,  $b_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$

x	y	xy	x <sup>2</sup>
1	2.5	2.5	1
2	3.5	7	4
3	5	15	9
4	6.5	26	16
5	7	35	25
<b>15</b>	<b>24.5</b>	<b>85.5</b>	<b>55</b>

y	6
2.5	0
3.7	-0.2
4.9	0.1
6.1	-0.3
7.3	0
<b>0</b>	

$b_0 = 1.3$   
 $b_1 = 1.2$   
 $\therefore y = 1.3 + 1.2x$

Now let us do an example here to you know clarify this you know theory, of least square method. Let us consider that some experimental value in general we are considering that experimental value as you know independent variables like x where x values are like suppose 1, 2, 3, 4, and 5.

And this x value will you know effect this dependent values like y which will be valued as 2.5 for x 1. Similarly 3.5 for x 2 and it will be you know here 5. Let it be 5 for x 3 and then it will be 6.5 for 4 and 7 for value x 5. Now in this case you have to find out you have to fit this you know data and proposing that equation y is equal to b 0 + b 1 into x.

Now based on this experimental data, you have to find out this  $b_0$  and  $b_1$  value. Now we have to use those you know equivalent to calculate this  $b_0$  and  $b_1$ . So what is that equation? We know that  $b_0$  that will be is equal to what?

Summation of  $y_i$ , summation of you know  $x_i$  square and then minus summation of  $x_i$  summation of  $x_i y_i$  divided by you know that  $n$  into you know summation of  $x_i$  square minus of summation of  $x_i$  whole square. This is your  $b_0$ .

Whereas  $b_1$  will be is equal to  $n$  into summation of  $x_i y_i$  minus summation of  $x_i$  into summation of  $y_i$  divided by  $n$  into summation of  $x_i$  square minus you know summation of  $x_i$  whole square. So in this way you can calculate what will be the  $b_0$ . So as per this first of all you have to find out what will be the summation of  $y$ , what will be the summation of  $x_i$  square, what will be the summation of  $x_i y_i$ .

So let us find out those you know values. Here let it be  $x$ , here let it be  $y$ , here let it be  $xy$  value and then  $x$  square and then here you can say after that you can easily calculate. So what is the  $x$  value here 1, here 2, 3, 4, 5. These are the  $x$  values and  $y$  values are here 2.5, here 3.5 and 5 and 6.6 and 7. And then  $xy$  that is  $x$  into  $y$  it will be coming as 2.5.

And then 7 here and then it will be 3 into 5 15, then 4 into 6.5 it will be coming 26 and then 5 into 7 35. And then  $x$  square it will be coming as what is the value of  $x$  square here. This will be 1 here then 4 this 9 and then here 16 and then 25. Now we have to find out the summation of this  $x$ .

This will be coming as 15 and summation of  $y$  it is coming as 24.5 and summation of  $xy$  it is coming 85.5 and summation of  $x$  square it will be coming as 55. After that, you just you know calculate what should be the value of this  $b_0$  and  $b_1$ . So what should be the  $b_0$ ? After substitution of this value here in this equation, we can get  $b_0$  is equal to 1.3 and  $b_1$  is equal to 1.2.

So from this you know example we can say that from this experimental data of  $x$  and  $y$  we can find out what will be the  $b_0$  and  $b_1$ . Now final equation then it will be coming as here  $y$ . That will be is equal to  $1.3 + 1.2$  into  $x$ . So this will be your

proposed equation based on your experimental data and by this equation you can calculate what will be the y value once you know that x value.

Suppose that you know that x value is 1. Then what should be the y value. So it will be coming what is the value? Let it be 1, so  $1.2 + 1.3$ . Then it will be simply 2.5. So as per this equation as per this equation of predicted value, so it will be coming as 2.5. Whereas if you consider that x is equal to 2, you will see that this value will be coming as per this equation, it will be coming as 3.7. Whereas, here y value is 3.5.

So we are getting from this equation it is coming 3.7. There will be a certain deviation, very small deviation will be there. Whereas the first point, it is exactly the same as with the experimental data. Similarly, if suppose x is equal to 3, you can get this value or the value it is coming 4.9 whereas, experimental value is 5. So there is also small deviation.

Similarly, if you are considering that x is equal to 4, experimental value is 6.5 but your predicted value by this equation it is coming 6.1. Similarly, for x is equal to you know 5 we are getting this y value as 7.3 whereas its value as per experiment, it is 7. So there is a deviation.

So we can say there will be a certain deviation for each value of this experimental value comparing with that, you know predicted value. So those errors in this case first point this error is coming 0, second point it is coming -0.2. Third point it is coming 0.1 this error and fourth point is -0.3 and last point it is coming almost what is that 0.

And you will see that error is coming almost you know that here is 0. So you are getting here zero error and equation what is proposed it is exactly giving the same value of experimental data without you know that considerable you know error.

So we can say that we can predict we can propose an equation, where we will be considering there will be a certain you know that coefficients that is to be found from the experimental data and how to find out that experimental data you can use this least square method.

Now how you know what is the extent of goodness that is R square value what should be that value, you have to find out based on this experimental data now for that you need to calculate as per discussion that what should be sum squares.

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Sum Squares

$$SS_{xx} = \sum (x_i - \bar{x})^2 = 10$$

$$\bar{x} = \frac{1}{n} \sum x_i = 3$$

$$SS_{yy} = \sum (y_i - \bar{y})^2 = 14.7$$

$$\bar{y} = \frac{1}{n} \sum y_i = 4.9$$

$$SS_{xy} = \sum (x_i - \bar{x})(y_i - \bar{y}) = 12$$

$$SE(b_0) = s \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{SS_{xx}}} = 0.332$$

$$SE(b_1) = \frac{s}{\sqrt{SS_{xx}}} = 0.1$$

$$r^2 = \frac{SS_{xy}^2}{SS_{xx} SS_{yy}} = \frac{12^2}{10 \times 14.7} = \frac{144}{147} = 0.98 \approx 1$$

$$s = \sqrt{\frac{SS_{yy} - \frac{SS_{xy}^2}{SS_{xx}}}{n-2}} = 0.314$$

$y = 1.3 + 1.2x$  is fitting very well with the experimental data.

So sum squares if you consider here sum squares, let us see what is the sum square are here. First of all SS xx to be calculated thus will be equal to what? This is basically x i minus x bar what should be the value here? But for that you need to know that x bar where x bar this is basically that 1 by n into summation of know that x i.

So it is coming as per that data it is coming 3 and then SS xx after substitution of this x bar and subtracting that x bar from that individual data of x i and then whole square of this data and then summing up it will be you know giving the value n. Similarly, Ss yy to be estimated. This will be basically defined as Y i minus Y bar again whole square, this will be coming as what?

But before calculating you have to first calculate what will be the Y bar. So this is basically 1 by n into summation of Y i. So it is coming as here 4.9. So after substitution of here, this SS yy it will be coming as 14.7. And then you have to calculate what should be the R square value. So R square value that is correlation coefficient it is basically, what is that, defined as SS xy square divided by SS xx into SS yy.

So for this  $SS_{xy}$  also it is required to know. So  $SS_{xy}$  can be obtained based on this you know definition here, that is  $\sum (x_i - \bar{x})(y_i - \bar{y})$ . So after substitution of this value, you can get this value as 12. Now after substitution of this value of  $SS_{xy}$  is nothing but 12. So 12 square divided by  $SS_{xx}$  it is basically 10 and  $SS_{yy}$  it is 14.7.

So it is coming as 144 divided by 147 it is coming 0.98. So it is very near about to 1.

So we can see that this equation  $y$  is equal to that means  $1.3 + 1.2x$  is fitting very well. very well with the experimental data. So this is your final you know proposed equation here. So in this way we can obtain what should be the you know goodness of fit there that is  $R$  square value correlation coefficient.

And then you know what will be the standard error based on that  $b_0$  value, standard error that will be is equal to as per that  $b_0$ . So it will be basically  $s$  into square root of  $\frac{1}{n} + \bar{x}^2$  divided by  $SS_{xx}$ . So it is coming basically 0.332 after substitution of this value and SE based on  $b_1$  it is coming  $s$  by root over  $SS_{xx}$ .

It is coming 0.1 where  $S$  is basically square root of  $SS_{yy} - \frac{SS_{xy}^2}{SS_{xx}}$  divided by  $SS_{xx}$  divided by  $n - 2$ . So after substitution of this value, it is coming 0.316. So we can obtain this standard error based on these coefficients  $b_0$  and  $b_1$  based on this equation.

So we you know that, then consider an equation like in this format of  $Y$  is equal to  $b_0 + b_1x$  and if you know that experimental value of  $x$  and  $y$  then you can easily hone that or propose that equation in the form of  $Y$  is equal to  $b_0 + b_1x$  just to and also obtain that  $b_0$  and  $b_1$  from this experimental data.

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## Fitting non-linear equation by making it as linear form

Non linear equation	Linear equation : $Y = a + bX$	Make
$y = ax^2 + b$ ✓	$Y = aX + b$ $Y = b, a \leftarrow b_0$	$y$ as $Y$ , $X^2$ as $X$
$y^2 = a/x + b$	$Y = aX + b$	$y^2$ as $Y$ , $1/x$ as $X$
$1/y = a(x+3) + b$	$Y = aX + b$	$1/y$ as $Y$ , $(x+3)$ as $X$
$\sin y = a(x^2 - 4)$	$Y = aX + b$	$\sin y$ as $Y$ , $(x^2 - 4)$ as $X$ , $b$ as $0$
$y = 1 + x(mx^2 + n)^{1/2}$	$Y = aX + b$	$(y-1)^2/x^2$ as $Y$ , $x^2$ as $X$ ; $m$ as $a$ and $n$ as $b$
$y = ax^b$	Take logarithm on both sides i.e. $\ln(y) = b \ln(x) + \ln(a)$ implies $Y = aX + b$	$\ln(y)$ as $Y$ , $\ln(x)$ as $X$ , $\ln(a)$ as $b$ and $b$ as $a$

Now another important point that for different chemical engineering operation, you may get different forms of you know experimental data and you will see that that experimental data may come you know based on different you know dependent independent variables.

Now that dependent variables maybe in terms of frictional pressure drop, maybe you know some you know combined form of frictional pressure drop and with other you know variables and as a whole one dependent variables would be formed based on you know combination of other variables.

And also you will see that the independent variables maybe of different forms. So you need to sometimes correlate to those independent and dependent variables and to predict those dependent variables based on independent variables, you can you know rearrange those variables or you can propose those, you know experimental data based on that equation of the form that is linear form of that is  $Y$  is equal to here  $b_0 + b_1x$ .

But sometimes you will see that some general you know principles, general equations that are coming from that basic laws. There also you will see that some laws will be in other forms of that you know  $b_0 + b_1x$  function. There maybe like you know the format like  $y$  is equal to  $a x^2 + b$ .



There may be you know that some other forms  $y$  square is equal to  $a$  by  $x$  plus  $b$ . There may be you know that some forms will be coming as  $1$  by  $y$  is equal to  $a$  into  $x$  plus  $3$  plus  $b$ . This type of form. Maybe you know  $\sin y$  will be equals to  $a$  into  $x$  square plus  $4$  or  $x$  square minus  $4$ . Sometimes you will see some forms will be coming as  $y$  is equal to  $1$  plus  $x$  into  $m$   $x$  square plus  $n$  whole to the power  $2$ .

Or sometimes you will see that some equation will be coming as you know power law likewise equal to  $a$  into  $x$  to the power  $b$ . So those equations are you know that nonlinear form it may be but single equation nonlinear form. So to fit those nonlinear form of equation with the experimental data, what we have to do?

You have to first convert this nonlinear equation into a linear form. After that you just follow this least square method to find out that unknown coefficients based on those equation. So let us see here, what are the different types of equation you may expect there. Like here  $Y$  is equal to  $aX$  square plus  $b$ .

If suppose this type of equation is coming, and you have to find out what should be the value of  $a$  and  $b$  here of this equation. Here  $x$  square or  $x$  is you know independent variables and  $y$  is dependent variables. So this is nonlinear equation. You have to you know rearrange this nonlinear equation into a linear equation. How to do that?

If you consider that this equation will be is equal to  $Y = aX + b$  or you can say that  $Y$  will be is equal to what?  $b$   $1x + b$   $0$ . So in this case, what we have to do this  $Y$  to be considered as capital  $Y$  as a dependent new equation, new variables and  $x$  square will be considered as  $X$  here. So here in this case, you can get this  $Y = aX + b$ .

Now comparing this equation of  $Y = b$   $1x + b$   $0$ . So as per least square method, you can easily find out this here  $b$   $1$  and  $b$   $0$  based on your experimental data of  $x$  and  $y$ . Similarly,  $y$  square will be equals to  $a$  by  $x$  plus  $b$ . You just you know rearrange this as  $y = aX + b$  where in this case capital  $Y$  would be is equal to simply  $Y$  square.

And here  $X$  will be is equal to what  $1$  by  $x$ . So this then again you have to compare with this equation and then follow that least square method that what we have discussed here. Similarly, suppose if you are having this type of equation or you want

to propose this type of equation with your experimental data and fit this equation with your experimental data.

Now to find out this unknown variables of a and unknown coefficient of a and b here, what you have to do? You have to make it linear form as  $Y = aX + b$ . Like in this case you have to consider here 1 by y would be is equal to Y and  $x + 3$  will be as X. And then you just fit it with your experimental data and follow this least square method.

Similarly, siny that will be is equal to a into x square plus b or x square minus b. So in this case again siny to be considered as capital Y here and x square minus 4 will be considered as X and then simply it will be coming as  $Y = aX + b$ . This is basically that equation. Similarly,  $y = 1 + x$  into mx square plus n whole to the power half.

This is basically again you can write in this form  $Y = aX + b$  where very complicated here in this case, y minus 1 whole square divided by x square will be as in Y whereas x square will be as X. Here see important thing is that dependent and independent variables combinely you know that they can form one dependent variables here as Y.

So here see Y and X here both as a combined they are forming one dependent variable as  $y - 1$  whole square by x square. And it will be regarded as here Y. And then x square will be as X. So again, if you are having this type of form and then follow this least square method as discussed here, you can get what will be the value of a and b there.

And once you know that a and b and then you can consider that here m should be as a and n should be as b. Here again if suppose, if you want to you know fit this equation of Y is equal to  $aX$  to the power b. This is you know power law model. What you have to do to make this you know linear form you have to take the logarithm on both sides of this equation like here  $\ln y$  that will be is equal to b into  $\ln x$  plus  $\ln a$ .

This will be simply  $Y = aX + b$  where Y will be is equal to here  $\ln y$  and X will be here  $\ln x$ . And a and b are as accordingly they are a will be is equal to b here, b will be is equal to  $\ln a$ . So in this way you can calculate or you can say that here b will be

is equal to here b 1 and ln a will be is equal to b 0. So accordingly you can calculate here.

So in this way you can you know make that nonlinear to linear and then comparing with this you know equation of b 1 plus b 1x plus b 0 and then apply that equation of least square method to find out this b 1 and b 0 value. Now let us consider one example here based on this you know nonlinear equation

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Example

$f = f(Re)$

$f = a Re^b$

$Re$	$f$
4000	0.01
4496	0.01
4999	0.009
5497	0.009
5997	0.009

$Re = \frac{\rho u d}{\mu} < 2300$   
 $> 4000$

$\Delta P_f = \frac{2f \rho u^2 L}{d}$

$f = \frac{\Delta P_f d}{2 \rho u^2 L}$

$Re_{crit} f = \frac{16}{Re}$

$f = 0.079 Re^{-0.25}$

Where we can consider here one example of like let us consider there is an operation like oil is flowing through pipe. Now during the flow there will be some frictional pressure drop and from that frictional pressure drop you have to calculate what will be the friction factor there, friction factor as part principles of fluid mechanics there.

That whenever there will be frictional pressure drop now you have to you know, know what should be the friction factor based on which you can say that, that flow will be how viscous and all those things. Now this friction factor is basically a function of Reynolds number.

What is that Reynolds number we have discussed at the very beginning of this course that Reynolds number is a dimensionless number, which is defined as you know  $\rho u d$  by  $\mu$ .  $\rho$  is the density of the fluid,  $u$  is the velocity of the flow and also  $d$  is the diameter of the pipe and  $\mu$  is the you know viscosity.

So whenever pipe is there and through the pipe is fluid is flowing like oil, water whatever it is. Then you will see that there will be some frictional pressure drop between these two points, point 1 and point 2. So this frictional pressure drop, from this frictional pressure drop, there will be some factor, friction factor it is called.

That friction factor it is coming basically this frictional pressure drop is depending on the you know that kinetic energy of the system and then the factor of that you know kinetic energy to be you know that, you know resulted from this friction factor and will be equal to that kinetic energy for which you have to you know multiply some factor it is called friction factor.

Now that friction factor, you know more about that frictional pressure drop, friction factor improved mechanics course there. We have already, you know developed one course that MOOC course that is fluid flow operations. There you I think will know more about this friction factor and frictional pressure drop.

There we have already you know floated you know you can also have those you know lectures in you know in YouTube also there. Or you can you know register for this course in future also if it is coming then there. And you will know that more about that frictional pressure drop and friction factor.

Now this frictional pressure drop or friction factor, that friction factor is basically is defined as what is that this friction first friction factor, this frictional pressure drop first it is basically you know  $2f$  into  $\rho u^2 L$  by  $d$  okay. So from this you can calculate what will be the  $f$ . This is basically  $\Delta P f d$ ,  $d$  is the diameter of the pipe.

This is  $d$ ,  $d$  by  $2 \rho u^2 L$ . From this, this is basically  $L$ , this distance is  $L$  and diameter is  $d$  and density of the you know fluid is  $\rho$  and you know that viscosity is  $\mu$ . So you know now this friction factor is basically depending on the Reynolds number.

Now you will see that, if Reynolds number is value is less than 2300 you will see this you know flow will be laminar, very slow flow of this you know there and highly viscous manner will be there and because of which there will be a flow is very, you

know slow and it is called laminar flow and if Reynolds number is greater than 4000s it will be called as you know turbulent flow.

So basically this friction factor depending on the you know Reynolds number. For laminar flow Reynolds number is you know you know for laminar flow, this friction factor is  $16$  by Reynolds number. Whereas for turbulent flow, this friction factor is you know  $0.079$  into Reynolds number to the power  $-0.25$ . So this is your friction factor.

Now this  $0.079$  and  $0.25$  those values are actually unknown values. Those are obtained based on the experimental data. Now let us consider this type of you know correlation. Let us consider that this  $f$  will be is equal to here some value of  $a$  into Reynolds number to the power you know  $b$ . Now in this case, this friction factor is a you know function of Reynolds number and it is correlated by this equation.

So this is nonlinear equation, you have to find out this  $a$  and  $b$  from your experimental data. Now how to do that experiment? First you have to do this experimental to find out this frictional pressure drop and from that frictional pressure drop, you have to calculate what should be the you know friction factor and then Reynolds number.

You will see that based on that Reynolds number this friction factor will be changing. Now let us consider those values here. Now if you have this Reynolds number and friction factor like this, for Reynolds number of 4000s this friction factor is coming  $0.01$  sorry  $0.01$ , this is your friction factor for this Reynolds number.

And for Reynolds number 4496 this friction factor is  $0.01$  whereas 4999 this friction factor is coming  $0.009$ . Whereas for Reynolds number 5497 it is coming  $0.009$  and then for Reynolds number 5997 it is coming  $0.009$  up to here three digit we are considering. Now based on these you know experimental data you have to establish this equation  $f$  is equal to  $a$  into  $Re$  to the power  $b$ .

You have to find out what will be the  $a$  and  $b$ , this coefficient based on this experimental. So you have to you know follow that least square method. Let us do this here.

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$$f = a Re^b$$

$$\Rightarrow \ln f = \ln a + b \ln(Re)$$

$$y = b_0 + b_1 x$$

$$y = \ln f, \quad x = \ln(Re)$$

$$b = b_1, \quad \ln a = b_0$$

$$x = \ln(Re) \quad y = \ln(f) \quad xy \quad x^2 \quad \epsilon \quad (x - \bar{x})^2 \quad (y - \bar{y})^2 \quad (x - \bar{x})(y - \bar{y})$$

What you have to do first, you have to convert this equation  $a$  into Reynolds number to the power  $b$  to a linear form by taking logarithm on both sides of this equation as  $\ln f$ . That will be is equal to  $\ln a$  plus  $b$  into  $\ln$  you know Reynolds number. In this case we will consider here this  $\ln f$  will be is equal to  $Y$  and then  $\ln Re$  will be is equal to  $x$  and here  $b$  we will be considering as  $b_1$ .

And  $\ln a$  we will be considering as  $b_0$  and here thus plus. So we are having  $Y = b_0 + b_1 x$  where this  $y$  is equal to  $\ln f$  and  $x$  will be is equal to  $\ln Re$  and here  $b$  will be is equal to  $b_1$  and  $\ln a$  would be is equal to  $b_0$ . Now we are having this equation of linear equation from this nonlinear equation.

Now you have to solve or you have to fit this equation with your experimental data to find out this  $b_0$  and  $b_1$ . So in the same way you have to calculate all the values. As per that you have to calculate first what is the  $x$  value? This is basically  $\ln Re$ . You know  $Re$ , so what should be the  $\ln Re$ ;  $y$  this is basically  $\ln f$ .

You know that  $f$  value and accordingly it will be coming us  $\ln f$ . And then what is that. Here  $xy$  and then  $x$  square, like this and also epsilon  $a$ , epsilon here like this and accordingly you have to calculate also what is that you know that  $x$  minus  $x$  bar here whole square and then  $y$  minus  $y$  bar whole square and then here also  $x$  minus  $x$  bar into  $y$  minus  $y$  bar.

So for all those values here you can get different values of this xy, x square, epsilon, this and this.

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Handwritten calculations for linear regression parameters and R-squared value:

$$b_0 = \frac{\sum y_i \sum x_i^2 - \sum x_i \sum x_i y_i}{n \sum x_i^2 - (\sum x_i)^2} = -2.5436$$

$$b_1 = -0.24938$$

$$\bar{x} = 8.5066$$

$$\bar{y} = -4.665$$

$$SS_{xx} = 0.10$$

$$SS_{yy} = 0.006384$$

$$SS_{xy} = -0.02558$$

$$S = 0.001$$

$$R^2 = \frac{SS_{xy}^2}{SS_{xx} SS_{yy}} = 0.999$$

$$f = a Re^b$$

$$f = 0.079 Re^{-0.25}$$

$$\exp(b_1) = a = 0.0788$$

$$b = b_1 = -0.249 \approx -0.25$$

So after getting this xy and xy you can obtain this value of b 0 from that equation of here what is that summation of y i, summation of x i square minus summation of x i into summation of x i y i divided by what is that n into here summation of x i square minus summation of x i whole square. So after substitution of this value, it will be coming as - 2.5436.

Similarly, you can get after substitution of different value of xy summation in you know this equation of definition of b 1 it will be coming as -0.24938 and you can get x bar will be is equal to here 8.5066 and then y bar that will be is equal to minus here 4.665 and then SS xx you can get this value as you know that 0.10.

SS yy you can get this value of 0.006384 and then you can get a SS xy that will be is equal to -0.02558. And then you calculate S that will be coming as 0.001 and then finally after substitution of this some squares in the definition of R square then it will be coming as R square will be equals to here this is SS xx square, sorry this is xy square divided by here SS xx into SS x sorry yy. So it will be coming as 0.999.

So this is your correlation coefficient. So from this correlation coefficient you can obtain what will be the degree of fitness of this equation with your experimental data.

Since it is coming very near about to 1 we can say that this equation will be you know fitted exactly with that experimental data.

So finally we can get what will be the coefficient of you know a and b value and then what will be the final equation there. There in this case we can write then f will be is equal to simply what is that equation? F will be is equal to a into Reynolds number to the power b whereas a is coming as what is the value of a is coming?

It is coming as zero point you know that what is the value it is coming. This a is coming what is the value of this you know a value? A value will be is equal to what? Here a will be is equal to here exponent of b 0. This is exponent of b 0. This exponent of b 0 that means exp of b 0 that will be is equal to a. That is basically here you will get 0.0788 something.

So we can write 0.079 here into Reynolds number to the power. And b is basically here b 1. So it is coming -0.249. It is exactly -0.25. So it is coming as -0.25. So in this way you can have this equation. So we can develop this equation for f as here 0.079 Reynolds number to to power -0.25. So this equation is developed by Blasius when you know 1964.

So there they have developed this equation based on the experimental data. So how they have developed this equation basically, based on the experimental data and then following that least square method, what we have described here, exactly the same way.

So in this way you can also fit that experimental data and proposing that equation, linear equation like y is equal to b 0 plus b 1 x and you know fitting that equation with the experimental data, you can obtain unknown coefficients of b 0 and b 1 in this way. Now this is the simple way to you know fit the experimental data with the linear equation.

Now these things are basically for single equation. Now if there are more than one equation involving in a particular chemical engineering process, what we have to do. Like material balance, there are several units will be there in your chemical



engineering process. Now if you do the material balance you will see that there you may get more than two equations, they are even you know that with different you know unknown variables.

So there you may get that n number of linear and nonlinear equations. Let us consider first that material balance equation where you can get only linear equations, set of linear equations.

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The slide is titled "Set of linear algebraic equation". It contains a bullet point: "You may have a set of linear algebraic equations by material balance of any process. For that you will need to solve those equations for unknown variables. The equations can be organized as follows." Below this, three equations are listed:  $a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$ ,  $a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2$ , and  $a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n = b_m$ . Red lines underline the coefficients and variables in each equation. To the right of the equations are three red curly braces. Below the equations, it says "or in compact matrix notation" followed by the equation  $aX = b$  with a red circle around it. To the right of this is the text "There is a unique set of x's that satisfies Eq. (1)".

That set of linear equations can be expressed by this equation here given in the slides where this you will see that a 11, this is coefficient x 1 is one variable, x 2 is another variable and dot dot like n number of variables will be there. Now all those variables like suppose in a particular chemical process like distillation process.

So there are suppose you have to you know separate suppose, that propylene and benzene by distillation process. Now there are two components propylene and benzene. You have to heat it then in the vapor phase there will be some percentage of propylene and benzene and in the bottom phase, there will be a some percentage of benzene and propylene.

And you will see that there will be some total material balance will be there, like here what will be the you total amount of feed is coming into the distillation column and what is the output of that distillation column as overhead and bottom product. There you can get you know one total material balance equation.

And then if you consider individual components of suppose propylene and benzene and if you do the material balance for benzene and propylene in that distribution column, you will see that you can get two you know again equations. So you can get three you know equations there. All those equations will be linear equations.

So here simple equations, but in this case, you are having set of three equations with some unknown variables. So that you have to solve. Not only like this simple you know example you can get you know more than one unit distillation column along with you know that condenser, boiler, pumps.

Even other you know sometimes separation unit like adsorber, absorber, all those units, even sometimes reactor also can be used, like reactive distillation column. There separately reactor and distillation will be there. So in that case you will see that there are more than you know one units will be involving in a particular chemical engineering process.

So for that what you have to do? You have to do the material balance for all the units and then you can get the set of linear equations by balancing out those materials of that components in each you know unit. And you will get set of linear equations there. Now you have to solve those set of linear equations for unknown you know coefficients.

Like this if we express those you know equations by material balance as this format, okay? And then you have to you know solve this equations for this, you know unknown coefficients of like this a 11 to a mn. Now in this case, these are all you know linear equations here n number of you know variables involving there.

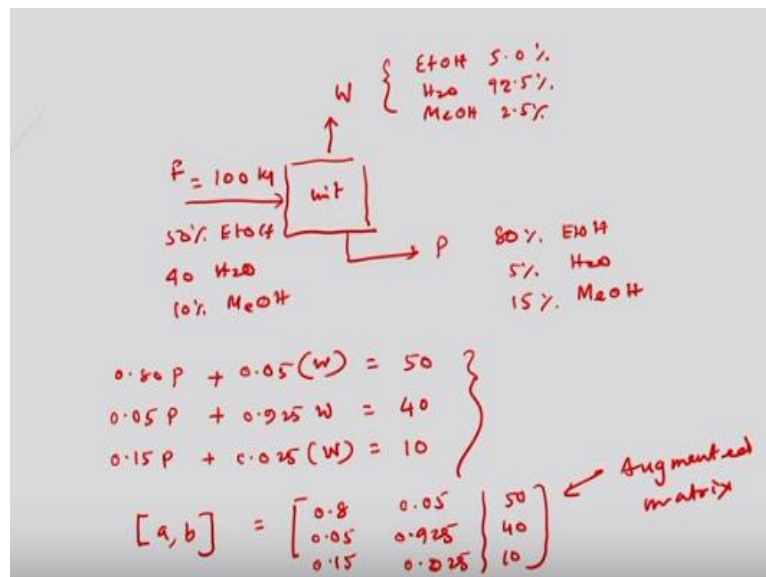
Like distillation there two variables here, what is that two components here propylene and benzene, here two unknown variables maybe there, they are fractions there you know more factions there. May be you know more than two variables also will be involving. Let be n number of variables like  $x_1$ ,  $x_2$ ,  $x_3$ .

Now you can get after material balance maybe more than two equations more than one equations and there may be considering there n number of equations can be formed by material balance. So you can express those set of linear equations after the material balance by this set of linear equations.

And in compact form you can express this set of linear equations by this  $aX = b$ . Where a will be a set of what is that a 11, a 12, nn and up to this a mn. And b will be like this these are the you know amount that is coefficients in this case. Like total material balance for the propylene or benzene or some components there.

So there it will be total what will be the amount in the inlet or outlet based on which this b 1, b 2, b m to be defined. So there is a unique set of this x's that satisfy this equation number one for which you can get the solution. So let us have an example for this you know concept.

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Let us have one chemical engineering unit here. In this case suppose in this unit some feed is entering as 100 kg as F and their composition is you know 50% you know ethanol and 40% water and 10% methanol. And they are after separation of this, you know component by you know either distillation process or other separation process let it be a general unit here, this is a separation unit.

And in this case we will see that some amount will be coming out as overhead that overhead will be you know as w which will contains that composition as ethanol as

you know 5.0% and here water will be as 92.5% and methanol here, it will be suppose 2.5%.

Whereas from the bottom product of the separation unit, it will be coming as P and composition as 80% you know ethanol and 5% water and remaining 15% will be you know methanol. Now in this case you have to you know write the set of linear equations for unknown variables here and express that, you know equations by material balance.

So if you do that material balance here, if we consider suppose ethanol first, we can write the ethanol balance here. Here one is input two outputs are there. Here we can write then input will be is equal to output since there is no reactions. So we can write for ethanol  $0.80$  as here as a product, this is  $0.80 P$  plus  $0.05 w$  that is output.

That will be is equal to input is simply 50% since 50 here. Similarly for you know that water balance if we do it will be coming  $0.05 P$  plus  $0.925 w$ . That will be is equal to amount of water entering. That will be 40 and similarly for methanol we can write  $0.15 p$   $0.025$  here  $w$ . That will be is equal to what, 10.

So these are the set of linear equations by the material balance. So we can simply express this material balance as a you know format of a, b that is matrix form here that will be is equal to like this 0.8, 0.05, 0.15 and then 0.05, 0.925 and then 0.025 and then here 50, 40, 10 this one. So this is called matrix form. It is called augmented matrix.

So in this way any chemical engineering process, you can represent the material balance equation a set of linear equations and after that you can solve either by you know computers by programming or you know software that is already given that you know programming language is their tools is there, so you can solve.

Or you can solve by manually also. You can use that Cramer's rule to solve that linear equation as a you know matrix format and you have to find out for the determinants and then how to find out that solution based on that Cramer's rule you can use okay. So I think you understood this you know computer techniques to you know how to

solve this to find out that you know nonlinear equation as a form of you know linear equation.

And then finding out the coefficient by least square method and also how to represent the, you know material balance equation for a particular chemical engineering process unit as a set of you know linear equation. And I would you know suggest to further reading of this know text books given here in the slides and practice it for understanding this you know this least square method.

And then you can try also with other  $y$  is equal to some you know some values of suppose  $a + b x$  or  $y$  is equal to  $mX + c$  format of equation just by having the values of you know  $x$  and  $y$  and then finding out the  $b_0$  and  $b_1$  as per that equation based on this least square method. So thank you for your attention.

Next lecture we will consider some nonlinear equation system and how to you know solve that nonlinear equations based on other you know principles.