Optimization in Chemical Engineering
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Lecture – 03
Introduction to Optimization
(Contd.)

Welcome to lecture 3 week 1. In week 1 we are talking about Introduction to Optimization. In today's class we will talk about examples of optimization in various engineering applications. So, basically we will go through some engineering applications where optimizations can be applied or are applied.

So, we will try to find out or we will try to understand what is the scope of optimization in such problems. In today's lecture we will not go into the details of problem formulations, we will do that in the next week. But in today's lecture we will take different engineering applications and I will try to understand the scope of optimization technique for these engineering applications.

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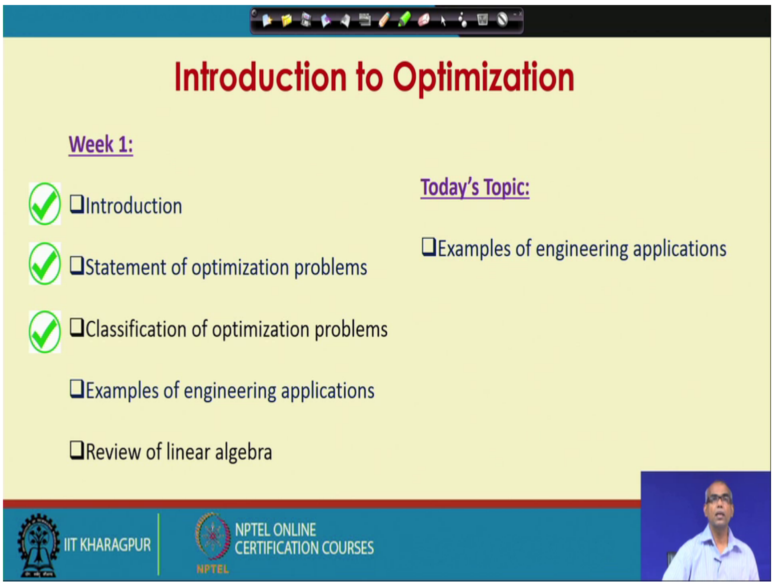

So, today's topic is examples of optimization or examples of engineering applications optimization in engineering applications.

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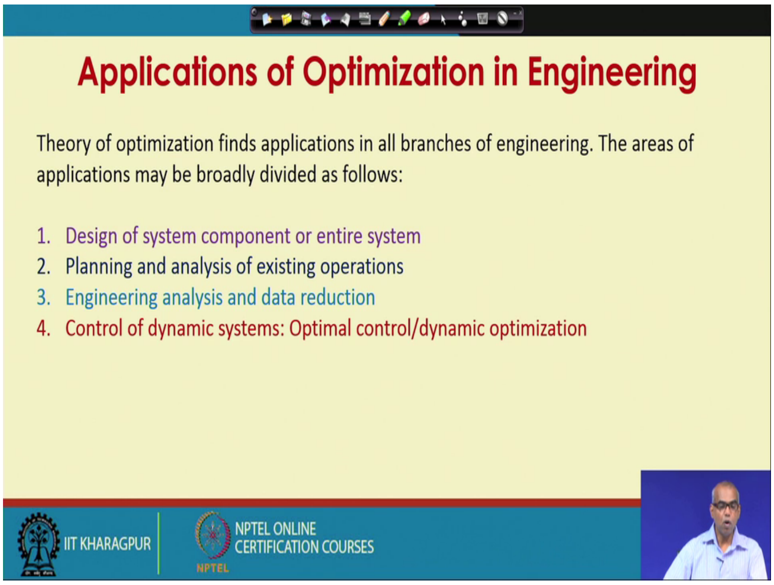

Theory of optimization finds applications in all branches of engineering. Various of applications may be broadly divided into four categories as follows, design of system components or entire systems. So, there are applications which will lie under the category of design of system components or the optimal design of the entire system.

Planning and analysis of existing operations engineering analysis and data reduction; So, engineering analysis of data and data reduction, control of dynamic systems, which leads to problems known as optimal control problems or dynamic optimization. This is another important class of problems in chemical engineering.

So, although this classification is not unique, all the possible engineering applications of optimization can be broadly classified or broadly categorized in these four different areas. So, design of system component or entire system, planning and analysis of existing operations, engineering analysis and data reduction, control of dynamic systems which is optimal control or dynamic optimization.

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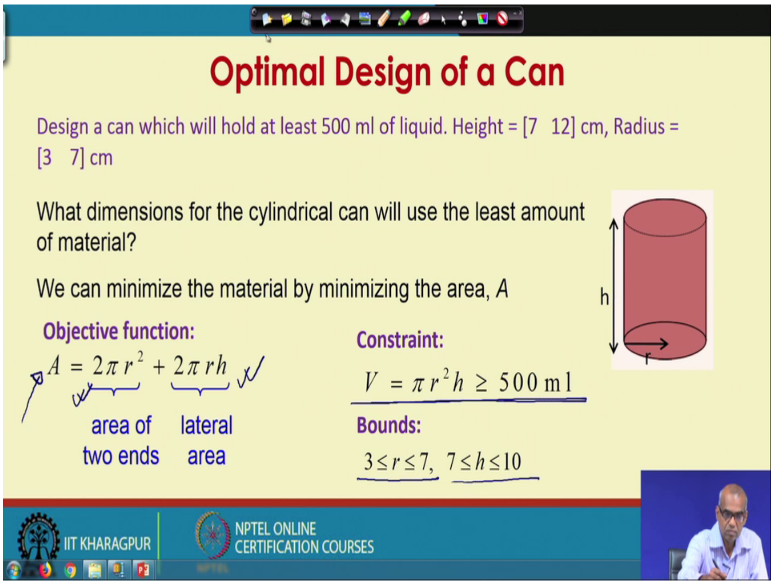

So, let us now take few examples and let us try to understand the scope of optimization or how the optimization can be applied in such problems or in such applications.

First let us take a simple example of optimal design of a can. So, we want to design a can. So, there are 2 decision variables, which we can vary and which we can find optimally. One is the diameter or radius of the can another is height of the can is a cylindrical can.

We are told that the height of the can be 7 centimetre to 12 centimetre and the radius may be anywhere between 3 centimetre to 7 centimetre. Here is a restriction on the design; we have to design the cylindrical can such that it will hold at least 500 m l of liquid. So, what is the scope of optimization, how the optimization will help.

So, the question that we are asking is what dimensions for the cylindrical can will use the least amount of material. And we can minimize the amount of material by minimizing the area. Because may be a metal sheet will be used to make the can to fabricate the can. So, what dimensions of the cylindrical can will be used which will hold at least 500 ml of liquid and will use minimum quantity of material so, that cost is minimum.

So, basically we want to find out the optimal values for the radius r and the height h that holds at least 500 ml of liquid; that means, the volume of the can is at least 500 ml and the cost is minimum. So, there is scope of optimization because we can find out minimum we can find out optimal values of r and h, which will minimize the cost. And to minimize the cost we can make use of the criterion that we have to minimize the area.

So, there are 2 areas curved area curve surface area as well as area of both the ends. So, we can find out the total area as follows. So, the objective function can be written as area which will minimize. So, area is a function of see a both r and h how. Area of 2 ends are both pi r square. So, 2 pi r square. So, this is the area of 2 ends and the lateral area or the curved surface area is 2 pi r h.

So, the objective function is A equal to 2 pi r square plus 2 pi r h. So, we have to find out the optimal value of r and h. So, that a is minimum, but we have a constraint; that means, the restriction on the design which says that the can must hold at least 500 ml of liquid. So, we calculate volume V as pi r square h and p i pi r square h must be greater or equal to 500. So, that is the constraint.

We have bounds on decision variables r and h. So, r will lie between 3 and 7 the height h will lie between 7 and 10. So, we have been able to identify the objective function the constraint as well as the bounds. So, thus the optimization techniques can be found out to find out the values of r and h that minimizes the total area a. So, there is scope for optimization.

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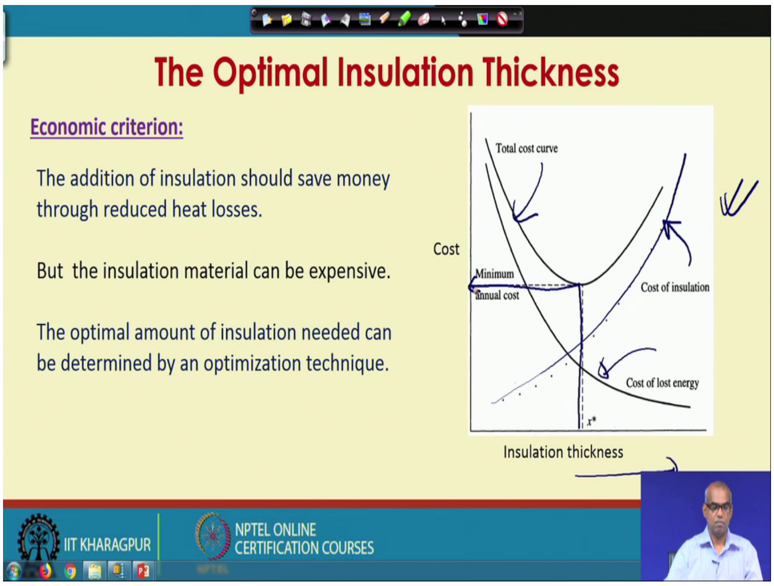

Next let us talk about optimal insulation thickness. You are familiar with this optimal insulation thickness; you have started this in your heat transfer course. Let us first talk about economic criterion. You know that addition of insulation will lead to reduced heat loss.

Loss of heat is equivalent to loss of money. So, the addition of insulation should save money through reduced heat loss, but the insulation material is expensive. So, we can go on adding insulation and by doing so, we will be reducing the heat loss and saving money on that, but at the same time we will be spending more because you have to buy more and more amount of insulation.

So, if you make a plot of cost versus insulation thickness as shown in this figure, you will see that as you increase the insulation thickness, the cost of lost energy will reduce because you will be reducing heat loss, but the cost of insulation will increase. So, if we add this 2 you will get the total cost curve and that total cost curve will show a thickness at which the total cost is minimum. So, at x star, at x star the cost is minimum. So, x star is the insulation thickness. So, there is scope of optimization.

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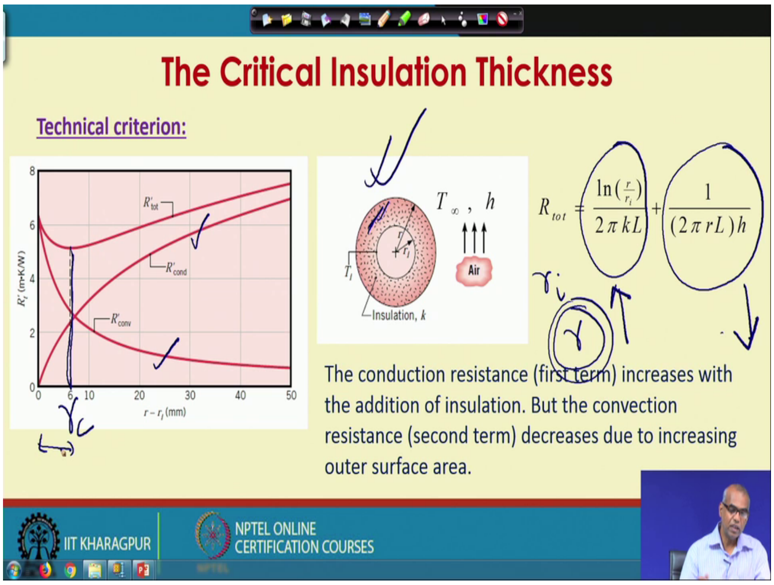

Let us now talk about the critical insulation thickness. Again you are familiar with this you have started this in your heat transfer course consider insulation is being added around a cylindrical tube and you want to reduce the heat loss. So, what you do is, you add insulation around the cylindrical surface. So, if you go on adding the insulation around the cylindrical surface, two things are happening. Look at this schematic; the inside circle corresponds to the inner pi and this is the insulation. So, let us consider r i as the radius of the pi and r is the radius of the pi after you have put insulation.

So, centre of the pi to the outer surface of the insulation that is r. So, as you go on increasing the insulation r increases. Now, to reduce heat loss we have to reduce we have to increase the total resistance. To reduce heat loss we have to increase the resistance assume increase. As we increase the insulation thickness as we increase the insulation thickness, the conduction resistance increases the conduction resistance is given by this you are adding more material. So, the conduction resistance increases.

But as you go on increasing the insulation material, you are also increasing the surface area the outer surface area. So, the convection resistance is decreasing. So, with increasing r, the conduction resistance is increasing, but the convection resistance is decreasing.

So, the conduction resistance increases with increasing thickness of insulation, but the convection resistance decreases with increasing insulation thickness. So, if you add up we will get how the total resistance changes with change in insulation thickness, and you see that there is a minimum at let us say r c which I call as critical insulation thickness.

So, up to critical insulation thickness between 0 to r c up to critical insulation thickness if you go on increasing the insulation, your resistance decreases. Beyond critical insulation if you add insulation the resistance increases. So, there is a good scope of optimization here, you need to know what is the critical insulation thickness.

So, up to critical insulation thickness, when I am adding the insulation my resistance decreases. So, heat loss increases. Say it may be desired for electrical wires, where you would like to dissipate the heat. But beyond critical insulation if you go on adding insulation, the total resistance increases. So, heat loss decreases. So, it may be desired for let us say putting insulation around steam pipes.

So, the knowledge of critical insulation thickness is extremely important and that can be found out by optimization technique.

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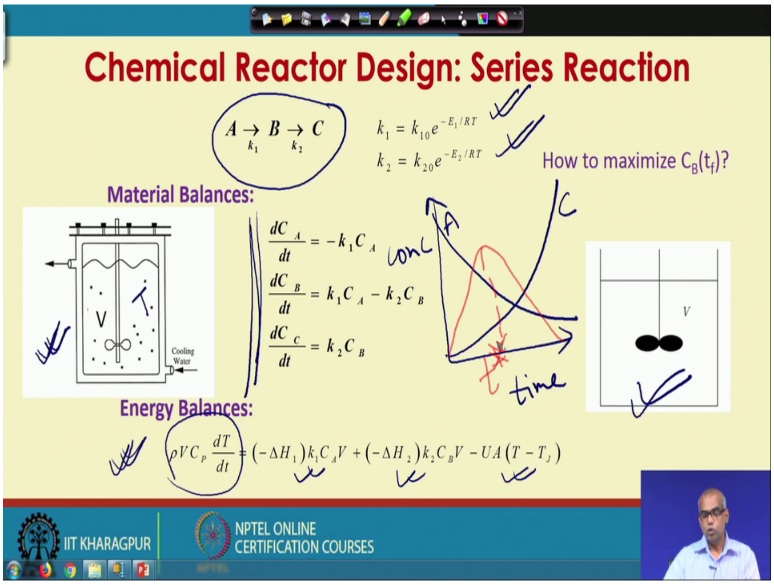

Let us talk about chemical reactor design a series reaction. So, this shows a typical batch reactor this also shows a typical batch reactor, but here, here we do not have a jacket around it, here we have a cooling water jacket around it by can by that you can control the temperature of the reactor.

Let us say inside this reactor, a series reaction takes place where the reactant A goes to B and B goes to C the reaction depth constants are given. The material balances on concentration of A B C are given they are simple mass balance equations. If we consider non isothermal operation, we have to write an energy balance equation non isothermal of if you have non isothermal operation; that means, we are also considering the temperature changes.

So, you have a cooling water jacket around the batch reactor and you can write the energy balance equation. The reactions may be exothermic so, you want to maintain a temperature within the reactor. So, the heat needs to be taken away and that can be done by circulating cooling water around the jacket.

So, the rate of term change of temperature inside the reactor can be written as heat generated due to reaction A to B, heat generated due to reaction B to C and heat removed by the cooling water. So, T J is the temperature of the cooling water in the jacket and T is the temperature of the reactor. So, these red constants these mass balance equation these energy balance equation constitute the process model. I want to maximize the amount of B at final time why is optimization required.

Let us try to understand intuitively, how the concentration of A B and C will change. So, I plot concentration versus time A goes to B. So, A only decreases C only forms. So, C increases, but what about B? If you look at a time at very early time, there will be little amount of B because not much of A has been converted to B, but if you wait for very long again you will get less amount of B, because most of the B has now converted to C.

So, the concentration of B will vary as it will increase reach maximum and there decrease. So, there will be a batch time corresponding to which there will be maximum amount of B. So, T star is that optimal time which can be found out optimally. So, again there is a good scope of optimization here.

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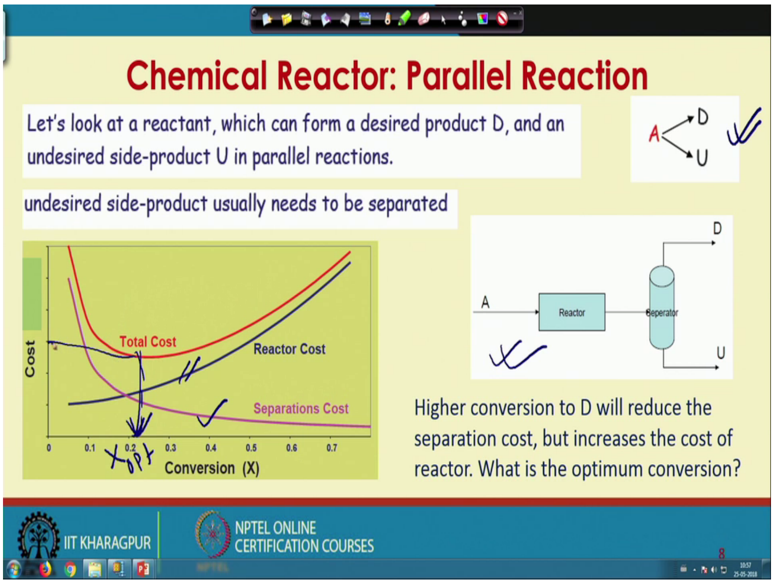

Another example from chemical reactor; this time instead of series reaction let us consider there is parallel reaction. Let us look at a reactant, which can form a desired product D, and an undesired side product U in parallel reactions like this, undesired side product usually needs to be separated.

Now, higher conversion of A to D will reduce the separation cost, but higher conversion of A to D will require increased cost of reactor. So, as the conversion increases the separation cost decreases because you need to separate less, but as the conversion increases the reactor cost also increases. So, if you add this up, you have the total cost and total cost shows a minimum corresponding to a conversion, which is optimum conversion. So, you can find out optimally the optimum conversion at which the total cost is minimum. So, we have to see that there are conflicting natures. So, while you are increasing conversion your separation cost decreases, but reactor cost increases. So, there will be an optimal conversion at which the total cost will be minimum.

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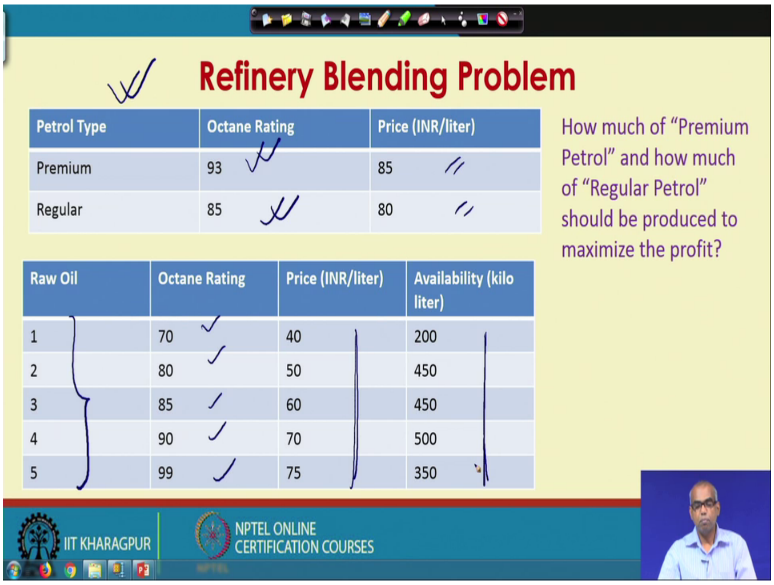

Let us next talk about a blending problem, a refinery blending problem. There is a refinery, which makes two types of petrol's premium petrol and regular petrol by mixing 5 different types of crude oil or raw oil. The premium petrol and the regular petrol have octane rating. So, the octane rating must not exceed 93 for premium petrol and 85 for regular petrol their prices are given. Similarly each of this crude oils octane rating are specified, their price also specified and also in how much quantity these crude oils are available that are also specified.

So, the question is, how much of premium petrol and how much of regular petrol should be produced so, that the profit is maximized. So, this is an important problem important real life problem, which can be solved using optimization techniques and later on you will see that these class of problems leads to linear programming problem, where all your objective function will be linear and all the constants will also be linear.

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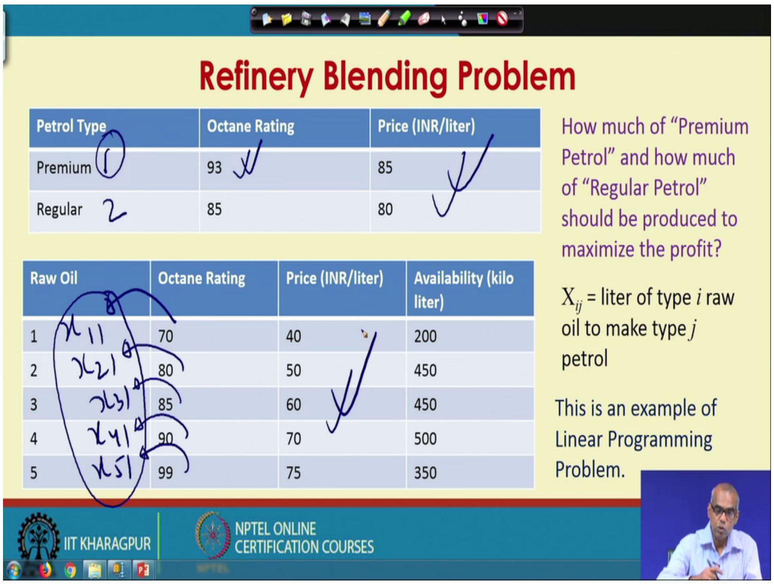

This is an example of linear programming problem. It will be clear to you later, but let us say you start thinking along the following direction.

You consider X i j litre of type i crude oil to make type j petrol. So, there are 2 types of petrol premium petrol and regular petrol. Let us call premium petrol as let say one regular petrol 2. So, X i j represents litre of type i raw oil to make type j petrol. So, x 11 x 1 2, x 1 x x 11, x 21, x 31, x 41, x 51 these are the quantities of the crude oils, which will make premium one petrol. So, 70 times x 11, 80 times x 21, 85 times x 31, 90 times x 41, 99 times x 51 divided by x 11 plus x 21 plus x 31 plus x 41 plus x 51 will not exceed 93 this is a constraint.

Similarly, you can find out all the constraints you see all that constraints are becoming linear in nature. Now, once you have these amounts, you can also have similar amounts for regular petrol type. Since the prices are given you can find out the profit. So, that will also be a linear equation. So, this will be an example of linear programming problem later on we will see how to solve it.

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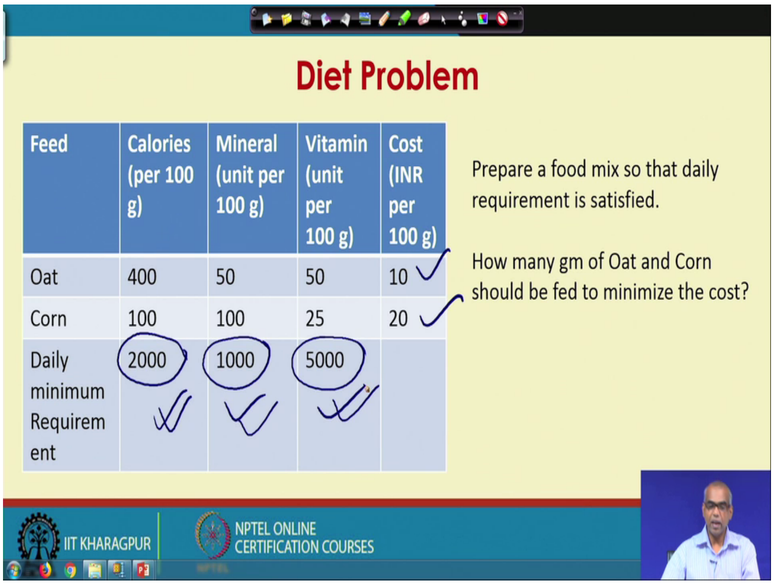

Another linear programming problem, which is of real life interest is the diet problem let us say you have to prepare a food mix so, that the daily requirement is satisfied and let us consider a very simple example, we are considering only 2 feed oat and corn.

The calories per 100 gram for oat and corn are given, minerals that are present in oat and corn are given, vitamin per unit vitamin in unit per 100 gram for both the feed are given, the cost are also given. And the daily minimum requirement is specified; that means, 2000 calorie per day is required, 1000 unit of mineral is required per day and 5000 unit of vitamin is required per day. Let us say this is this will be used as a cattle feed and the cattle's required these calories per day, these minerals per day, these vitamin per day.

So, the question I ask is how many gram of oat and how many gram of corn should be fed to minimize the cost. In the previous blending problem it was maximization of the profit, here it is the minimization of the cost.

So, you want to optimally, you want to find out optimal amount of oat and corn, which when mixed will minimize the cost, but at the same time the daily minimum requirement for the cattle as specified will be fulfilled. So, this is a diet problem again, this is a linear programming problem and important linear programming problem.

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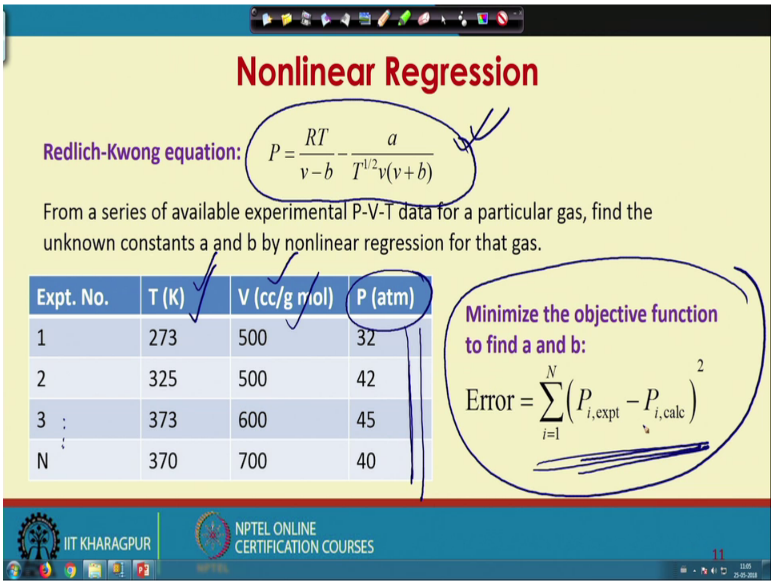

Next we will talk about non-linear regression. You know the ideal gas law P v equal to RT, you are also familiar with Redlich-Kwong equation, which is given as P equal to RT by v minus b minus a by T to the power half v into v plus b. In this equation there are 2 parameters a and b. From a series of available experimental pressure versus volume versus temperature data for a particular gas, we can find the unknown constants a and b by non-linear regression for that gas.

So, what is a scope for optimization? So, we do series of experiments 1 2 3 and then up to n. At different temperature and volume we have the pressures. So, these are experimental data and this pressure can also be calculated at these temperature and these volumes using this Redlich-Kwong equation. So, the difference between the experimental pressure and the calculated pressure is the error.

So, we want to minimize the error square. So, objective function will be the error square summed over all experimental data. Why square otherwise if you do not take square, you will get a wrong impression because some error may be positive some errors may be negative they can cancel each other out and they will not reflect the reality.

So, the better estimate will be you take error square. So, error square summed over all experimental data that is the total error, that must be minimized. So, you find out the optimal values of small a and small b which are the parameters of these, by minimizing this. So, this is there is a good scope of optimization and this is our non-linear regression can be done.

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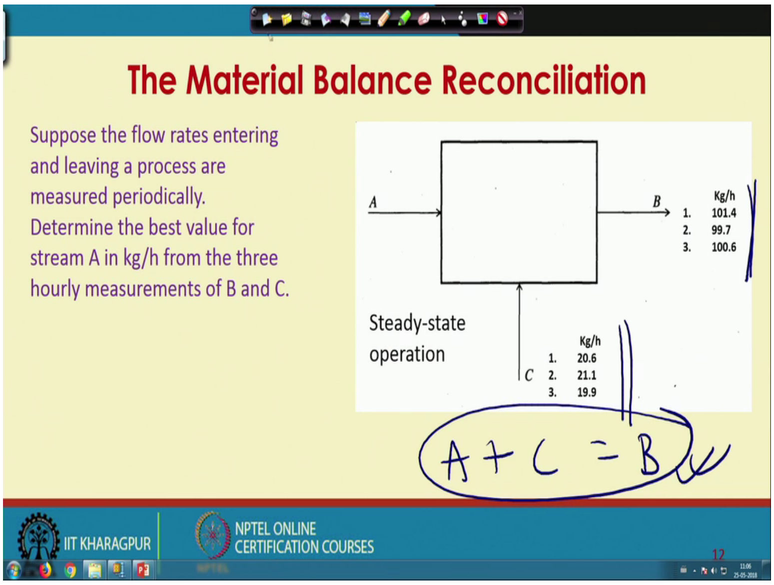

A close related problem is the material balance reconciliation. Suppose the flow rates entering and leaving a process are measured periodically, we want to determine the best value for the stream A in kilogram per hour, from the three hourly measurements of B and C is a steady state operation.

So, A and C stream enters, B stream leaves we have three hourly measured data. So, I want to estimate A, you know A plus C is equal to B because it is a steady state operation. So, we can make use of this to formulate an objective function and then optimization techniques can be used. So, let us see how.

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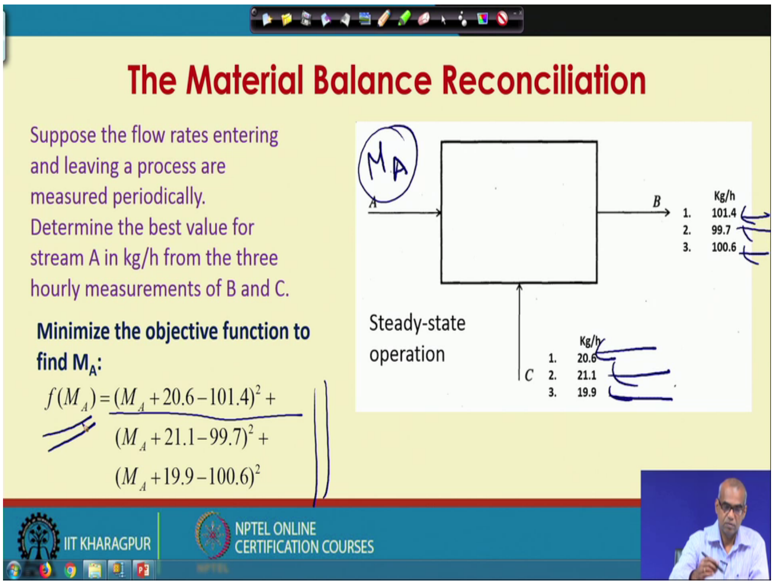

So, if the estimate of A is mass flow rate is M A. So, M A plus 20.6 will be equal to 101.4, similarly M A plus 21.1 minus 99.7 plus again similarly for the third data. So, ideally this would be 0. So, you have to minimize these objective function. So, that will be the best estimate for A mass flow rate of A.

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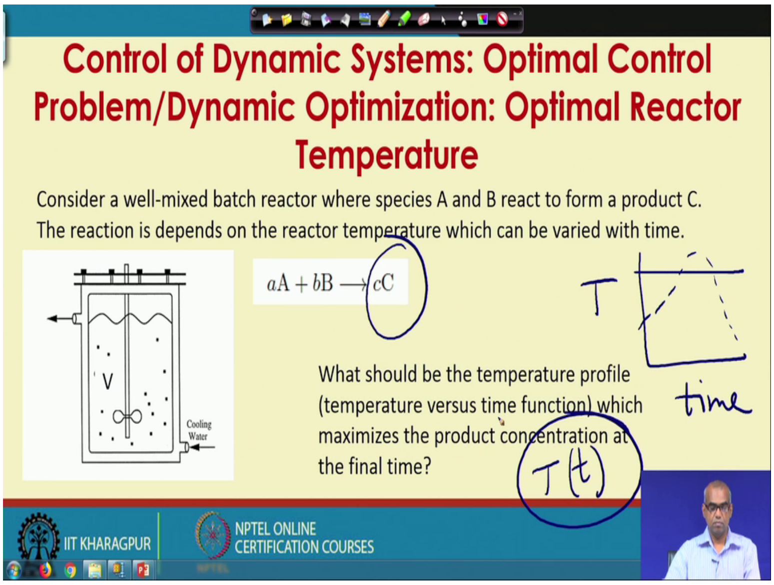

Now, will briefly talk about 2 special class of problems, known as optimal control problems or dynamic optimization problems.

First let us talk about optimal reactor temperature. Consider a well mixed batch reactor where species A and B react to form a product C. The reaction is dependent on the reactor temperature, and let us say you can vary the temperature at our will. So, the temperature influences the outcome of the reaction. So, the product how much of product will be formed will be depending on the temperature and the temperature can be varied.

So, the question we ask is, what should be the temperature of the reactor temperature will the temperature be constant or we have to follow of specific particular temperature profile. So, if I plot temperature versus time, will the temperature be constant throughout or maybe we can take let us say some kind of temperature profile, which will maximize the amount of C.

So, here basically the optimal solution is a function of time, you are finding out temperature versus time function, which maximizes the product concentration at final time, such problems are known as dynamic optimization problems.

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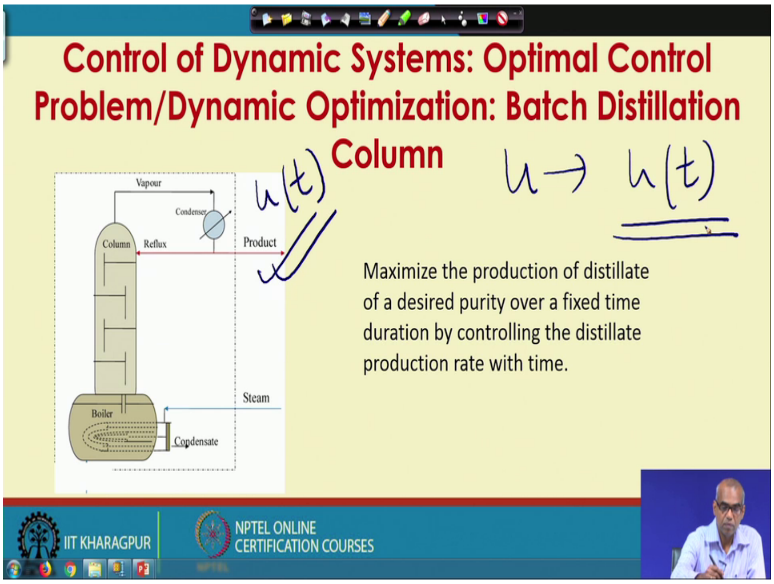

Still another example from batch distillation column; you can maximize the production of distillate of a desired purity over a fixed time duration, by controlling the distillate production rate with time. So, let us say the distillate production rate is say u t. So, u the production rate is the function of time.

So, how the production rate has to be changed with time so, that we can maximize the production of distillate of a desired purity over a fixed duration of time; this is also a dynamic optimization problem or optimal control problem. Such problems also appears in plug flow reactors, such optimization problems can also be formulated in fed batch fermentation processes so on and so forth.

With this we will conclude our lecture 3 here.