Optimization in Chemical Engineering

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Lecture - 02
Introduction to Optimization (Contd.)

Welcome to lecture 2 week 1; in this week we are talking about Introduction to Optimization. In lecture 1 we have talked about very briefly about optimization and we have talked that optimization is a mathematical technique to find out the best possible solution to your problem. So if optimization is a mathematical technique it is quite natural that the optimization problem will be stated in terms in terms of some standard mathematical form.

So in this lecture we will see what are the components of an optimization problem so that in later class we can formulate the optimization problem; so after talking about the various components of an optimization problem we will also briefly talked about the various classification of optimization problem that exist.

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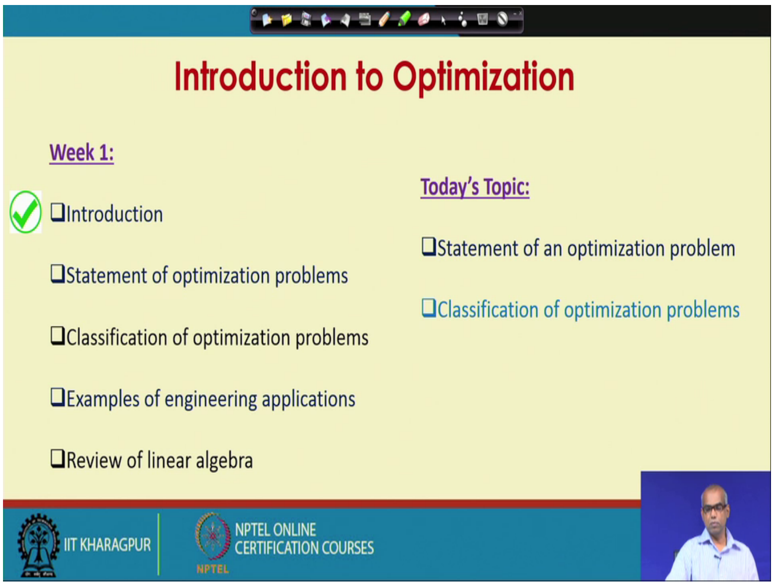

So, today's topic will be statement of an optimization problem and classification of optimization problems.

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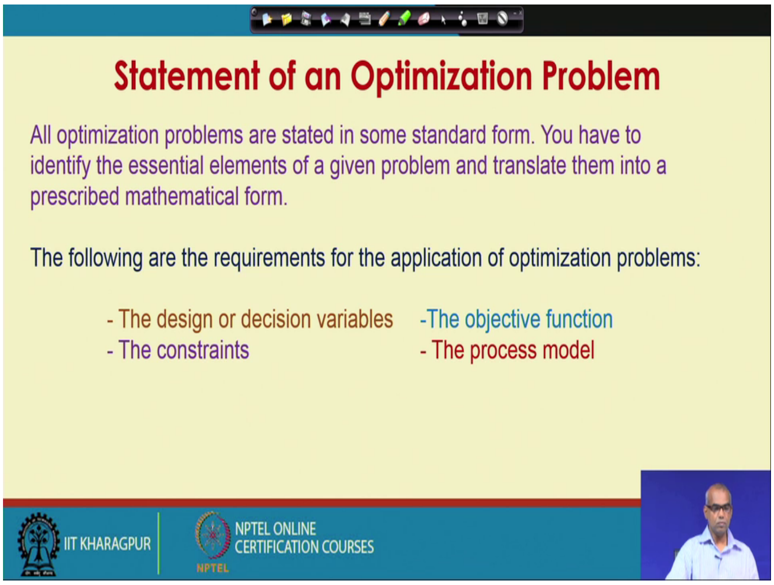

All optimization problems are stated in some standard mathematical form you have to identify the essential elements of a given problem and translate them into a prescribed mathematical form. The following are the requirements for the application of optimization problems the design variables or decision variables the objective function, the constraints, the process model. So you can perform a mathematical optimization if we assure or if you know how to formulate the objective function what are the decision variables how to formulate the constraints and maybe you may also require a process model that describes the behavior of the system under optimization.

So, now we will talk about the decision variables or design variables the objective function the constraints etcetera in some more detail.

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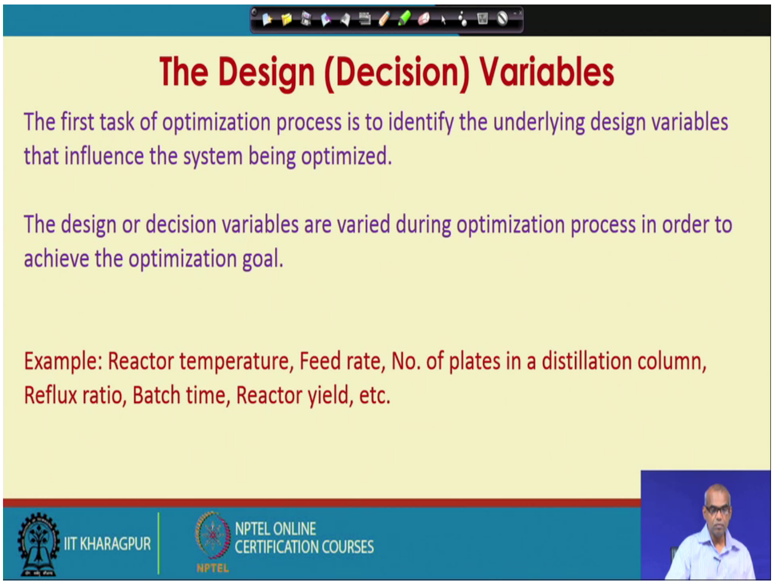

The first task of optimization process is to identify the underlying design variables that influence the system being optimized; so you need to know what are the variables that influence the system we are optimizing and you are trying to find out the optimal values for these variables, it may happen that some variables will influence the systems output or the systems response or the systems behavior to a large extend and there will be some variables which may be, but in sensitive meaning that those variables do not influence the behavior of the system much.

So, the variables which heavily influence the system will be consider as decision variables or design variables and the variables which do not influence the systems response that you are interested in may be consider at some constant level; that means, we can assign some constant nominal values to those variables. So this design variables or decision variables are varied during optimization process in order to find an optimal values of this variables so that we can achieve the optimization goal the optimization goals are usually say maximization of some profit or minimization of some cost this is in terms of economic consideration.

Later on we will see that we can also consider technical aspects and relate maximization and minimization problems; so some examples of design variables or decision variables may be you find the optimal reactor temperature, optimal feed rate, may be a constant feed rate or may be a feed rate profile; that means, the function of the feed rate with respective time; so feed rate may or may not remain constant with time number of plates in a distillation column, reflux ratio, optimal batch time, took maximize say product concentration, reactor yield etcetera.

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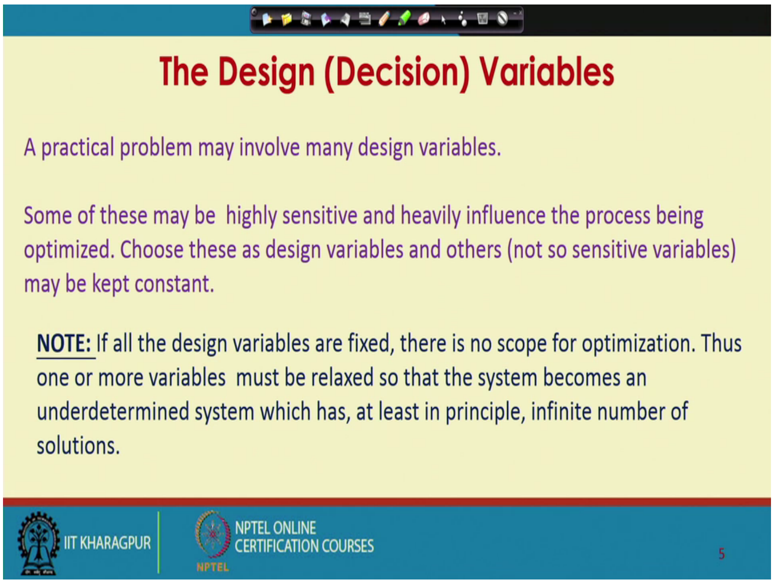

A practical problem may involve many design variables some of these may be highly sensitive and heavily influence the process being optimized we choose them as design variables and others which are not so sensitive variables may be kept constant at some nominal values. If all the variables are fixed then there is no scope for optimization thus 1 or more variables must be relaxed so that the system becomes an underdetermined system which has at least in principle infinite number of solutions.

So if all the design variables of a given optimization problems are fixed; then there is no scope for optimization because your system is completely defined and there will exist an unique solution to the problem. So for optimization to be possible we must have an underdetermined system so that in principle there will exist and infinite number of solution and the optimization technique will find out the best possible solution among several alternatives.

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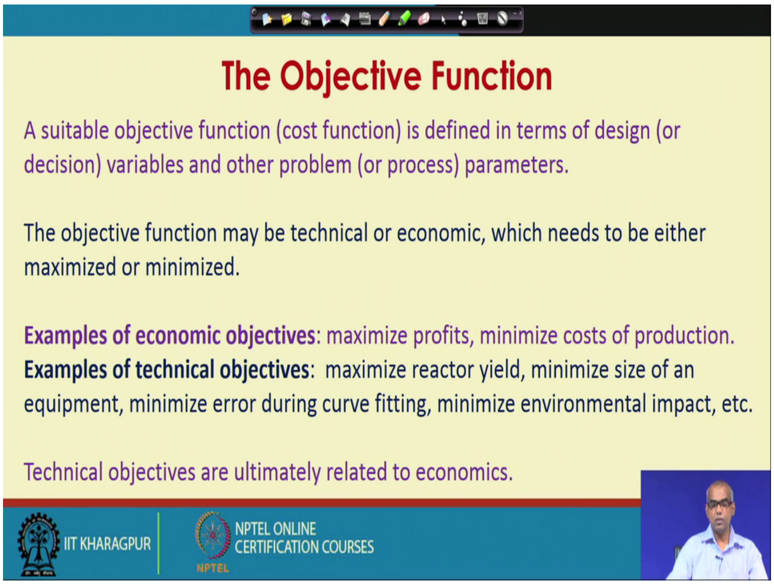

Next let us come to objective function; a suitable objective function also often known as cost function is defined in terms of design variables or decision variables and other problem or process parameters so the objective function or the cost function is a suitable function of design variables and other problem or process related parameters. The objective function may be technical or economic in nature which needs to be either maximized or minimized. Examples of economic objectives you want to maximize the profits for an operation you want to minimize the cost of production so you must formulate a function that tells you how much profit you will get and these profit expression will be a function of decision variables.

So, we will find out the optimal values of those decision variables that will maximize the profit similarly the objective function may also be minimization of cost of production so here also the cost of production will be a mathematical expression which is the function of decision variables. Examples of technical objectives; maximize reactor yield, minimize size of an equipment, minimize error during curve fitting, minimize environmental impact etcetera; remember in all the cases the objective function will be a function of decision variables. So we are going to find out the optimal values of the decision variables that maximize or minimize the objective function it can also be said that the technical objectives in an industrial operation will ultimately get reflected in economic objective function.

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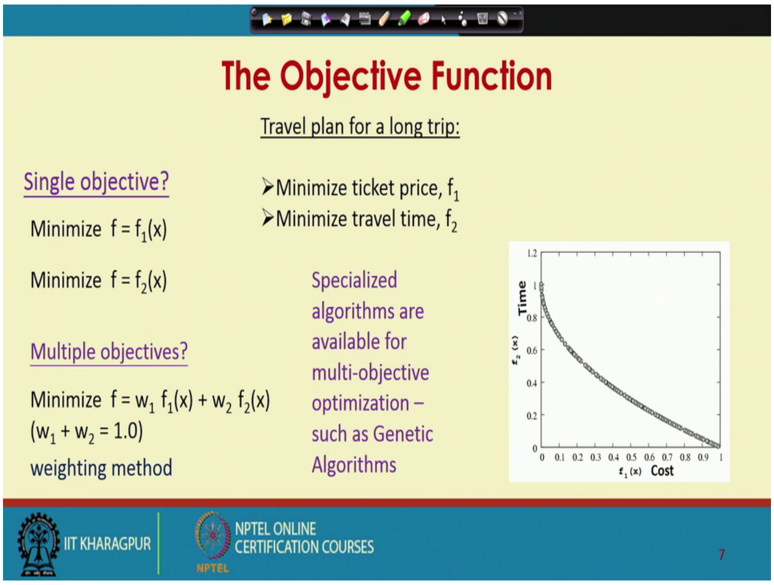

Let us consider a simple example and this will tell you that you may have single objective function, you may also have multiple objective function although in this course will essentially talk about optimization problems with single objective function. So let us consider a simple example of travel plan for a long trip so you are going for a long trip let us say very long trip, let us say you can take train or you can travel by air and you have different options there are flights which take less time than the others, but; obviously, the ticket price will be different. Similarly there are say super fast trains which will take less time unless say there are regular trains which will take more time, but again then the ticket price will be different.

So, if you want to optimize my travel plan, I may look for two things you can minimize the price of the ticket, you can minimize the travel time. If there is no restriction on travel time; obviously, I will try to minimize the cost of the ticket a money is no consideration I will try to minimize the travel time. So single objective optimization problem may be either minimize the ticket price that is f 1 or minimize the travel time that is f 2, but we perhaps will try to minimize both will try to minimize travel time as well as we will try to minimize ticket price.

But is this possible so if you plot cost; that means, ticket price versus travel time you see you get a plot like this; which says that if cost is higher the travel time is less if cost is more the travel time cost is less the travel time is more. So basically these two objectives conflict with each other; there are several real life problems where you have more than one objective functions and these objective functions conflict with each other such optimization problems are known as multi objective optimization problems. Although we will talk about only single objective optimization problems in this course there are several important real life multi objective optimization problems and specialized optimization tools are available for solutions of multi objective optimization problems; such as genetic algorithms. One way to solve a multi objective optimization problem is to convert it to a single objective optimization problem I can do that by taking weighted average of the individual objective functions and can formulate a composite single objective function and then can apply the single objective optimization techniques this is known as weighting method.

So, what I have done is I am taken a new objective function f which is w 1 into f 1 plus w 2 into f 2 so w 1 w 2 at different weights and w 1 plus w 2 equal to 1. So once I formulate this problem I can apply the techniques that will learn in this course for solution of optimization problem with single objective function, but please note that specialized techniques are available and for better solution you should applied those specialized algorithms for solution of multi objective optimization problems.

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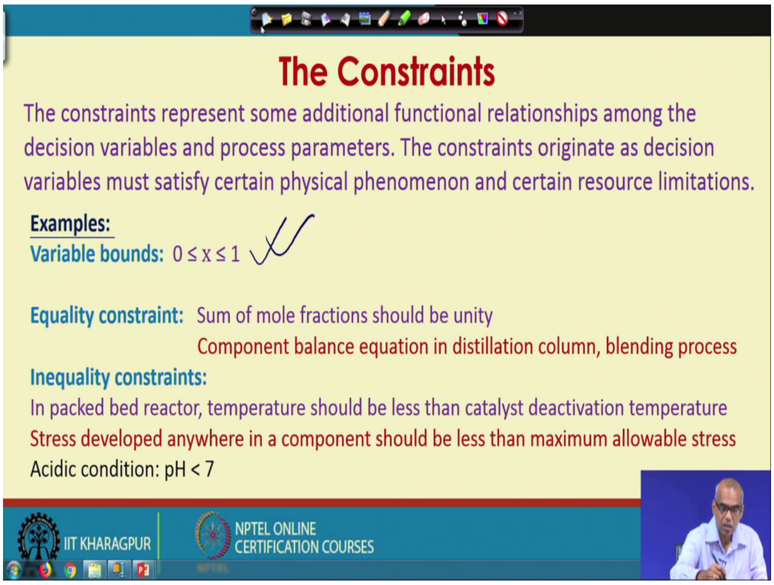

Next talk about the constraints; the constraints represent some additional functional relationships among the decision variables and process parameters. The constraints originate as decision variables must satisfy certain physical phenomenon and certain resource limitations. Let us now see what are the various types of constraints that will in counter with; so once again the constraints represents some additional functional relationship among the decision variables and the process parameters. So this is not an objective function this is a constraint function which is again a function of decision variables or other process related parameters. The constraints will appear because the decision variables must satisfy certain physical phenomenon or certain restrictions or certain resource limitations. Variable bounds the variable bounds is represented as if x is decision variable let us say x varies from 0 to 1 or x varies from 2 to 5 let us say the diameter of a can of a can that I am going to design will be lying in between 3 centimeter to 10 centimeter so we will write x is greater or equal to 3 less or equal to 10.

Equality constraints; so here the constraint function will be will have equality sign it will be an equalization; equality constraints that frequently appear in chemical engineering optimization problems are say some of mole fractions should be unity. Component balance equation in distillation column, component balance equation in blending process all these will lead to equations, so that is equality constraints. Inequality constraints will be of less or equal to type or greater or equal to type.

Note that less or equal to type can be to greater equal to type and vice versa by taking the minus sign, examples of inequality constraints in packed bed reactor; temperature should be less than catalyst deactivation temperature. So you can write temperature t must be less or equal to the temperature at which the catalyst becomes deactivated. Stress developed anywhere in a component should be less than maximum allowable stress; we will represent acidic condition as pH less than 7; so these are all examples of inequality constraints.

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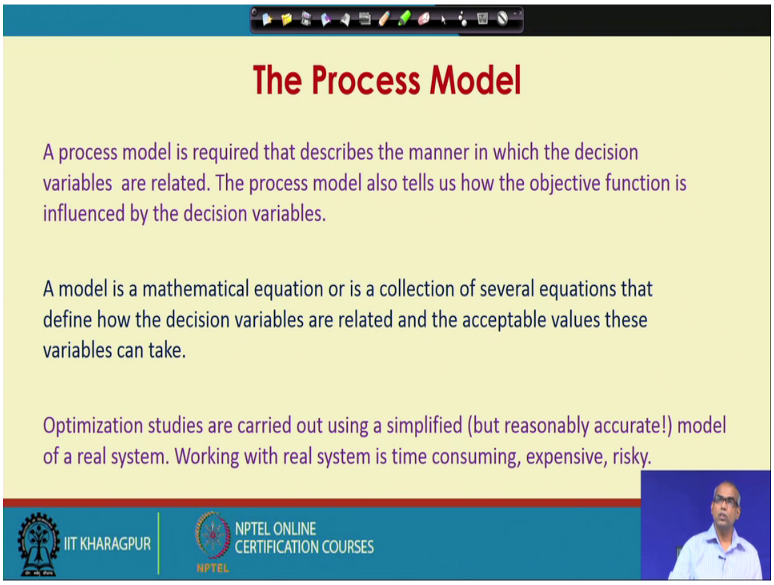

The process model; a process model is required that describes the manner in which the decision variables are related, the process model also tells us how the objective function is influenced by the decision variables. A model is a mathematical equation or is a collection of several equations that define how the decision variables are related and the acceptable values these variables can take. Optimization studies are carried out using a simplified, but reasonably accurate model of a real system working with real system is time consuming expensive as well as risky. So a realistic process model which represents the behavior of the system under optimization quit well is necessary for mathematical optimization to perform.

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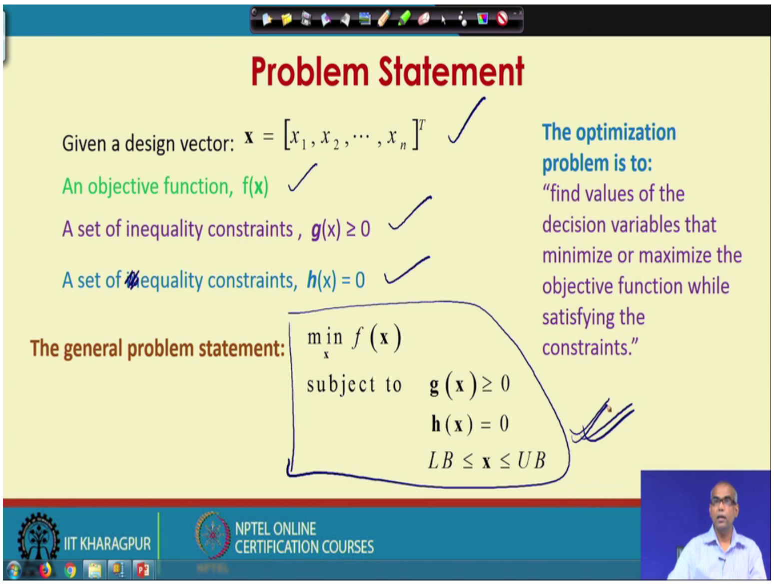

Now so we have seen that the components of an optimization problem are a decision variables, objective function, constraints. So given a set of design vector, given an objective function, given set of inequality constraint, given a set of equality constraint, the general problem statement will be you minimize function f x by finding out the decision variable x and decision variable x must satisfy the constraints inequality constraint g x grater or equal to 0, equality constraint h x equal to 0 and the bounds on decision variable x which is bounded between lower bound and upper bound.

In terms of words we can say the find the values of decision variable x that minimize or maximize the objective function while satisfying the constraints and this is the mathematical representation of a general optimization problem. So you have the design vectors or decision variable vectors x which may have n components x 1 x 2 up to x n; that means, there are n decision variables to be found out optimally. We have an objective function f x so the objective function is the function of the decision variable x we have set of inequality constraint g x grater or equal to 0, you have set of equality constraint h x equal to 0. Then the optimization problem segment is minimization f x subject to g x grater or equal to 0, h x equal to 0 and x is bounded between lower bound and upper bound.

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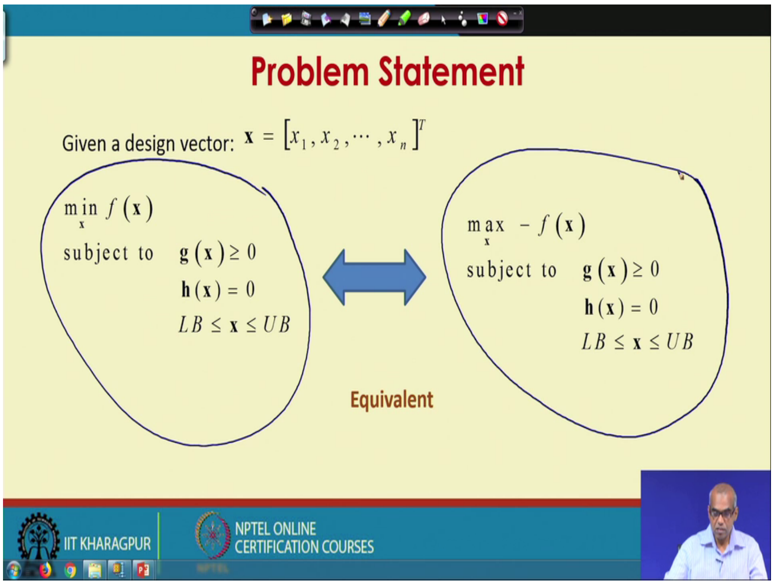

Note that the minimization of function f x and the maximization of minus f x is equivalent. So a general problem statement may be in terms of minimization of f x it may also be maximization of f x; because minimization of f x and maximization of minus f x are equivalent.

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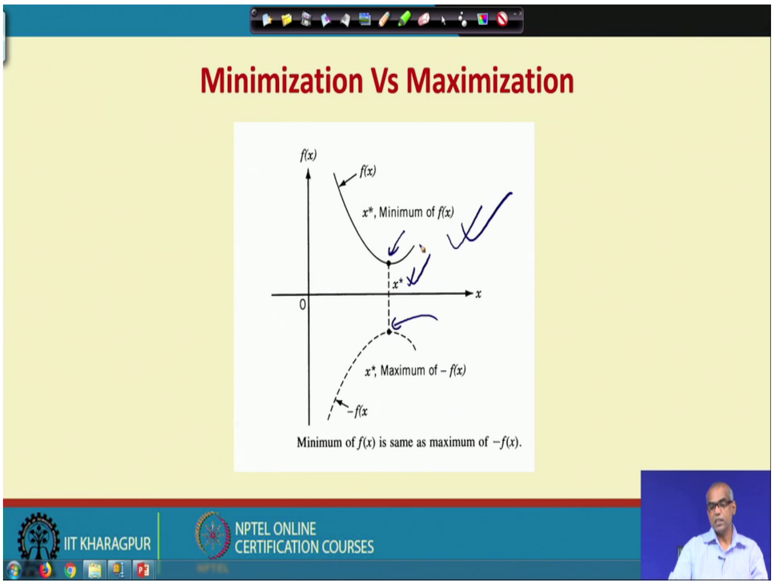

It can be clearly seen from here; so here I have plot a function single variable function f x you can see that a x star there is a minimum. If you now plot the function minus f x it will be the mirror image and the maxima will appear at the same value of x star; so minimum of f x is same as maximum of minus f x.

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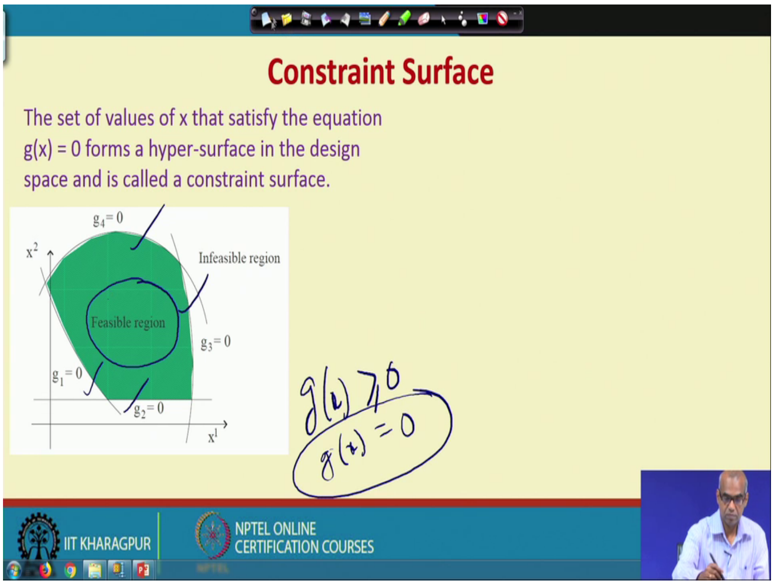

Next let us talk about constraints surface the set of values of x; that means, decision variables that satisfy the equation g x equal to 0 forms a hyper surface in the design space and is called a constraint surface so you have g x grater or equal to 0 as constraints. So now, let us see I have in this example I have 4 constraints g 1 g 2 g 3 g 4; see if plot this g x equal to 0 and the region that is bounded by g 1 g 2 g 3 g 4 these 4 constraints; that means, this green color is region is known as feasible region. So your optimal solution must lie within this region because the optimal solution has to satisfy these constraints; so we have to find out the optimal solution within this feasible region.

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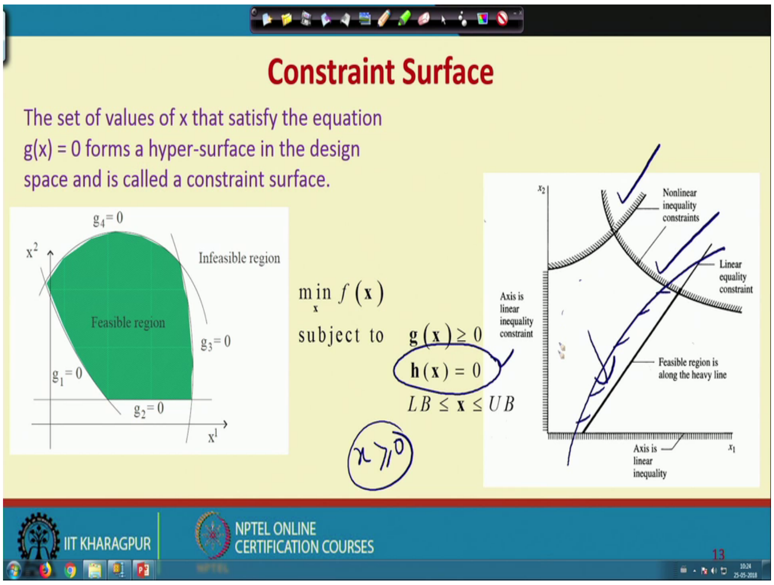

If I also have equality constraint; let us say here I have an inequality constraint g x grater or equal to 0, I have an another inequality constraint g x grater or equal to 0; x is a posses linear inequality constraint. So x grater or equal to 0 y grater or equal to 0 those x's are consider as linear inequality constraint and if I have an inequality constraint which is shown here the decision variables, the optimal decision variables or the optimal solution will lie in the feasible region.

If there was no equality constraint, but there was only say another inequality constraint like these this is your feasible region, but in the presence of equality constraint the feasible region is along these may be line which represents the equality constraint. So you must find the optimal solution along this line which is within the feasible region, but since the optimal solution has to satisfy both equality and inequality constraint it has to lie on the heavy line which represents the equality constraint.

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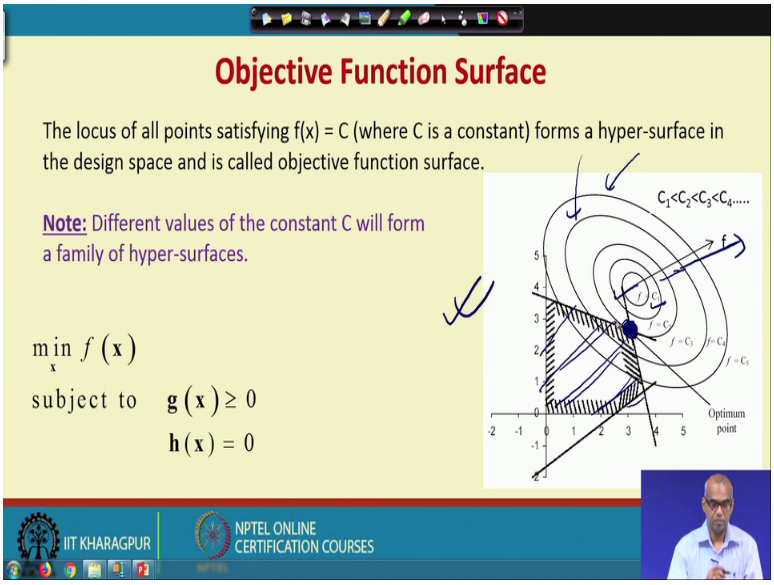

Objective function surface; the locus of all point satisfying f x equal to C where C is a constant, forms a hyper surface in the design space and is called objective function surface. So my objective function is f x so I assign different constraint values to the objective function f x equal to C 1 f x equal to C 2 f x equal to C 3 so on and so forth. And so if I do that this will form a hyper surface in the design space and this will be known as objective function surface. So different values of the constraint C will form a family of hyper surfaces which are known as objective function surface; look at the figure so these are objective function contours corresponding to f x equal to C 1 f x equal to C 2 so on and so forth.

As you go in this direction the value the objective function increases; that means, the innermost contours represents the minimum function value next is C 2 next is C 3 and maximum is C 4. I am I want to minimize this problem and let us say this is my feasible region, this hatched part is my feasible region. So the optimal solution lie within the feasible region and say this is the point which is which will lie in the feasible region and has the minimum value of the function objective function; see there exist this point there exist this point which has even less value compared to this point, but they are outside the feasible region so the optimum point is this.

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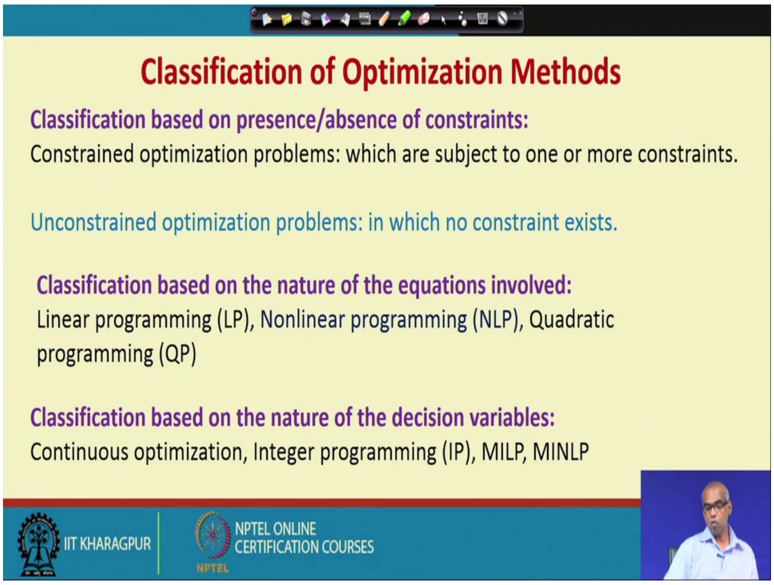

Next let us briefly talk about various classification of optimization methods or optimization problems; optimization problems can be classified in various ways one classification may be based on presence or absence of constraints. Constrained optimization problems are those which has one or more constraints, unconstrained optimization problems are those which do not have any constraints the classification of optimization problem may also be based on nature of the equations involved in case of linear programming problem the objective function is the linear equation all the constraints are linear equation.

In case of non-linear programming problem objective function may be non-linear the equations may also be non-linear, in case of quadratic programming problem the objective function is quadratic and the constraints are all linear, the classification of optimization problem may also be based on the nature of the decision variables. In case of continuous optimization problems the decision variables can take on continuous real values in case of integer programming problem the decision variables will take on only integer values.

In case of mixed integer linear programming problem you have a linear programming problem where the decision variables can take only integer values as well as real values; so mixed integer linear programming problem you can also have mix integer and non-linear programming problem here your problem is non-linear programming problem and the decision variables can take both real values as well as integer values. So some decision variables will be taking integer values, some decisions will be taking real values. So their MINLP, MILP and MINLP are also very important class of optimization problems in chemical engineering.

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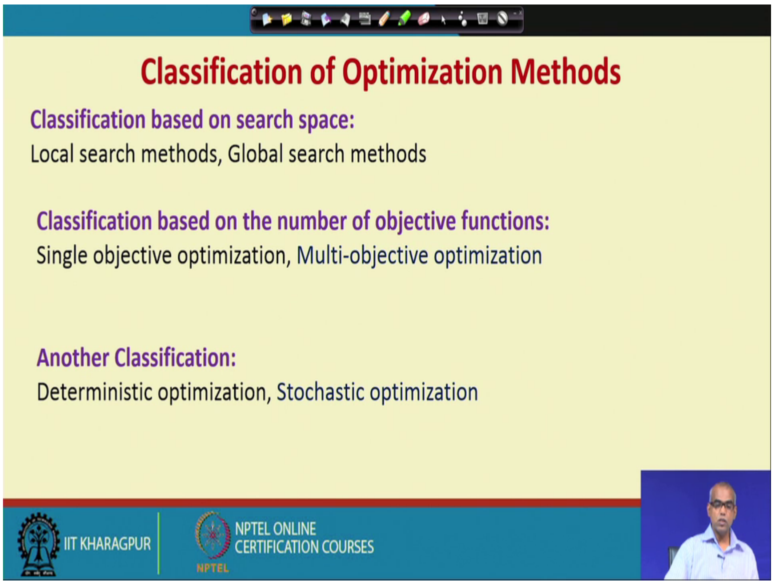

We can also have classification based on local search methods or global search method. So this will lead to local optimum or global optimum classification may be based on the number of objective functions we can have single optimization problems we may have multi objective optimization problems. Still another classification is possible based on whether the problem is deterministic in nature or there is an element of randomness which is known as stochastic optimization problems. So there are various classifications and there is no unique way of classifying them so based on various criteria you may have various ways of classifying the optimization problems.

With this we will stop here.