Optimization in Chemical Engineering

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Lecture – 06
Optimization Problem Formulation

Welcome to lecture 6 this is week 2 first lecture of week 2, in this week we will discuss about Optimization Problem Formulation. In our previous week we have discussed that optimization is a mathematical technique to find out the best possible solution. During the formulation of optimization problem, we need to write down or formulate the objective function and the constraints associated with the problem. While, you do this we need a mathematical description of the problem or mathematical description of the process that is under optimization.

So, the mathematical description of the process that is being optimized is known as a process model. So, in this lecture today we will first see process models and then we will talk about something called degrees of freedom analysis. And then in the later lectures of this week we will talk about various formulations, optimization problem formulations from different chemical engineering and biochemical engineering problems.

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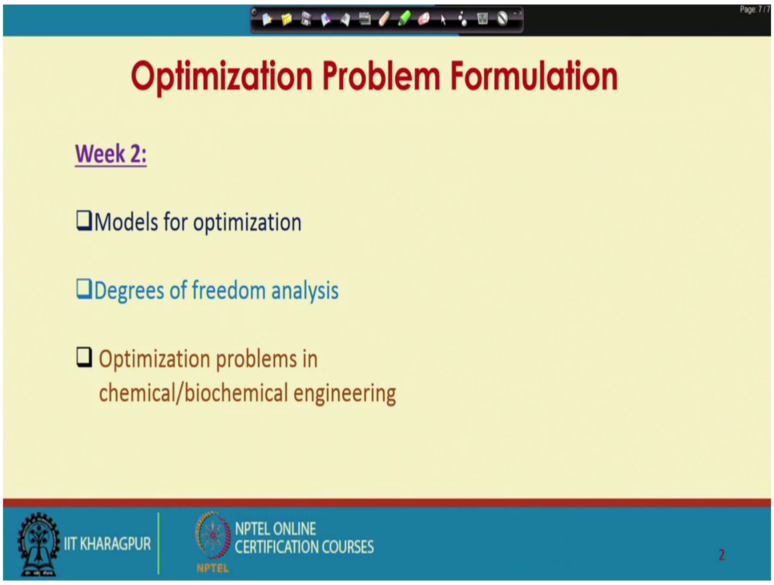

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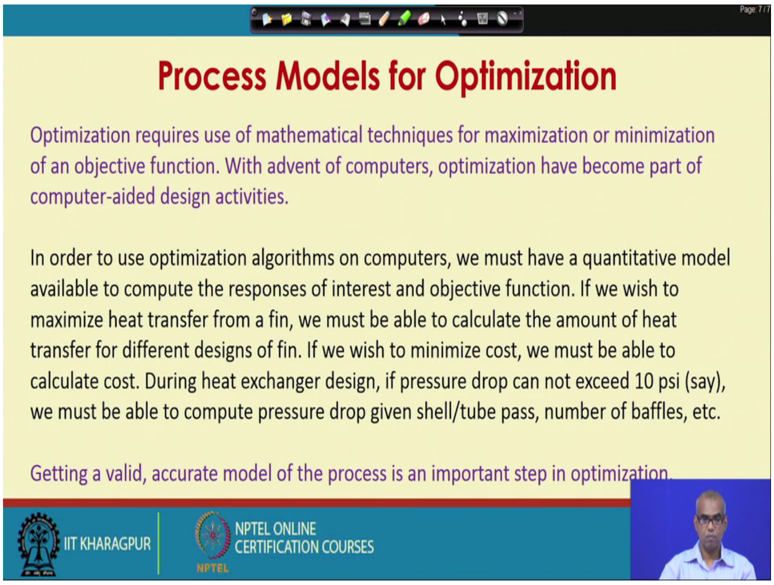

So, this is the agenda of week 2 we will see process models for optimization first, degrees of freedom analysis and then various optimization problem formulations in chemical biochemical engineering. Optimization requires use of mathematical techniques for maximization or minimization of an objective function. With advent of computers optimization have become part of computer aided design activities.

In order to use optimization algorithms and computers we must have a quantitative model available to compute the responses of interest and objective function, as well as constants associated with the problem.

If we wish to maximize heat transfer from a fin we must be able to calculate the amount of heat transfer from different designs of fin, if you have done a course on heat transfer you have studied heat transfer from fins. So, there are different designs of fins, so fins may have rectangular cross section, fins may have circular cross sections, triangular cross section, etcetera. So, if we have to design a suitable fin for our application and I want to maximize the amount of heat transfer from the fin by adopting different designs.

I must be able to calculate the amount of heat transfer that takes place from different designs. For example, what is the amount of heat transfer that will take place if I design a fin with rectangular cross section or what will happen if I design a fin with triangular cross section. So, we need a mathematical description of the fins performance and you have seen that the energy balance equation is used as a mathematical model for heat transfer phenomena in such cases.

Similarly, if we wish to minimize the cost of a process operation I must be able to compute the cost. Again let us say you are designing shell and tube heat exchanger and a constant has been imposed which says that the shell side as well as the tube side pressure drop must not exceed certain specified value, let us say 10 psi. So, I must be able to compute the pressure drop in the shell side and the tube side for a given design; that means, if I have chosen a certain length of tubes, shell diameter, number of baffles, etcetera pitch, etcetera. I must be able to compute what will be the pressure drop in shell side what will be the pressure drop in the tube side.

So, the set of equations or set of mathematical expression that will allow me to compute this is considered as model for the shell and tube heat exchanger. So, getting a valid and reasonably accurate model is very very important for successful application of optimization. So, if you look at this diagram first consider this in the box we have written process set of input goes from x 1 to x n to the process and these are the responses or output from the process which are y 1 to y k.

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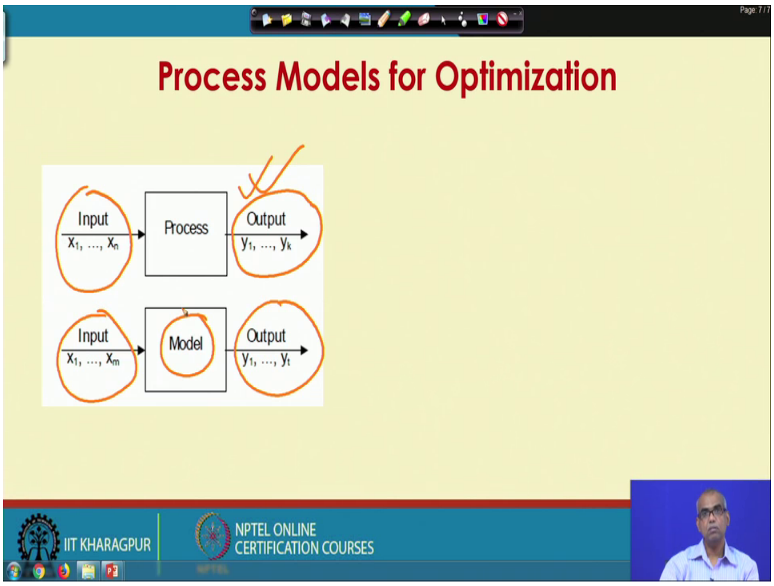

If I want to develop a model for the process what it means that I want to establish a relationship between inputs and outputs. It may not be necessary to consider all the inputs and all the outputs, because may be some inputs may be k types some fixed value and I may not be interested in some of the responses or outputs. So, if I choose certain inputs and corresponding outputs the relationship that exists between these input and this output is known as process model or model.

So, this model may be a simple algebraic equation, it may be a linear equation, it may be a series of linear equations, it may be some linear equations, some non-linear equations, it may be differential equation, set of differential equations coupled with some algebraic equations, it may be partial differential equations so on and so forth. Idea is that the process model will allow me to establish or to find out the responses of the process given a set of input, and this information is necessary during the course of optimization.

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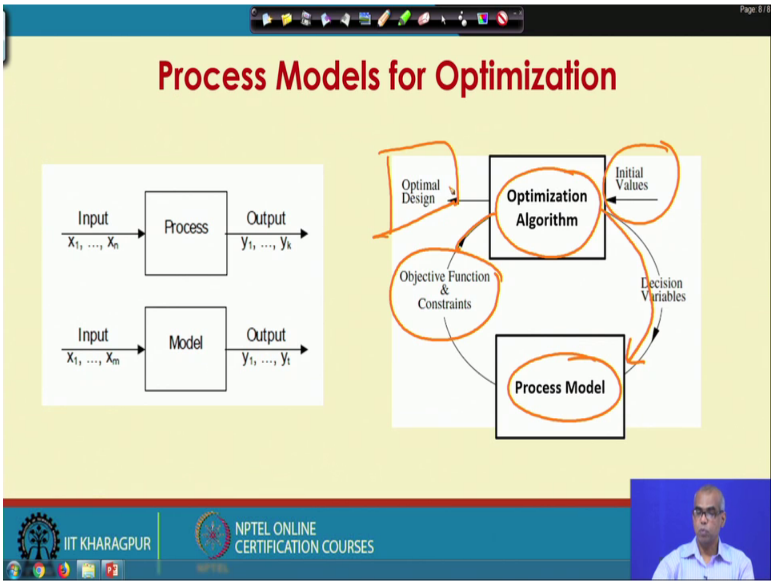

So, how a process model is useful in optimization is shown in this schematic. So, as we know now the optimization algorithms can be implemented and computed very easily this days, so we have this optimization algorithms. So, you start with some initial values for the optimal solutions. So, the decision variables goes to this process model which helps us to evaluate the objective functions, checks the constraints and again goes to the optimization algorithms.

So, the optimization algorithm iteratively uses the process model to find out better and better decision variables that maximizes and minimizes the objective function, while simultaneously satisfying all the constraints, and ultimately returns you the optimal solutions or optimal design for a design problem. So, this is how the process model is used during the course of optimization.

So, you are performing optimization on computers using optimization algorithms the optimization algorithms will call the process model iteratively, will pass on the trial solutions or the trial decision various set of decision variables to the process model. Process model will evaluate the objective functions check the constraints and it will be done iteratively. So, that the optimization algorithm converges to a set of decision variable which maximizes or minimizes the objective function and they also satisfy all the constants imposed on the problem.

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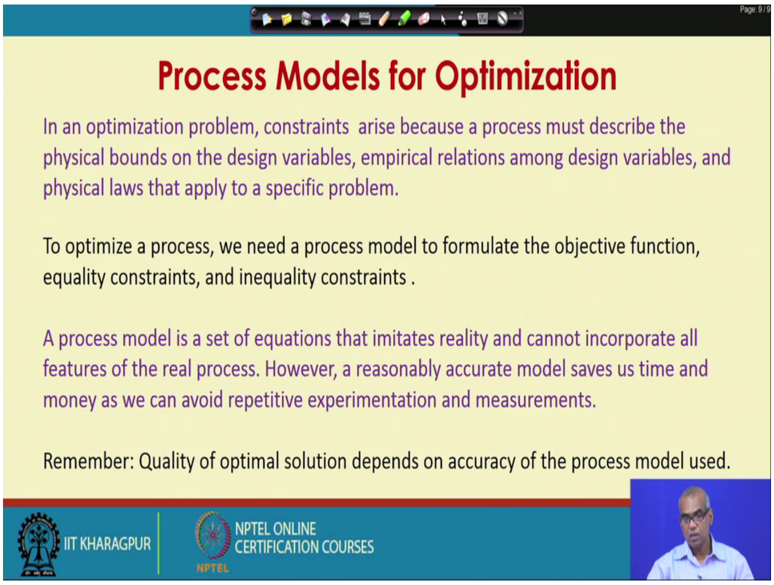

So, in an optimization problem constraints arise because a process must describe the physical bounds on the design variables. Empirical relations among design variables and physical laws that apply to a specific problem, to optimize a process we need a process model to formulate the objective function, equality constraints and inequality constraints.

A process model is a set of equations that imitates reality and cannot incorporate all features of the real process, that may not be possible because the real process may be extremely complex and it may not be possible by the set of equations that you are using to incorporate all the complexity that exist in a real process.

And also for optimization we would like to have a model which is simple, but we do not want to compromise much on the accuracy of the prediction by made by the model. So, we need a simple model, but reasonably accurate, if the model is very complex the optimization task may be very difficult, it may be extremely time consuming.

So, a reasonably accurate model is required. The process model saves us time and money as we can avoid repetitive experiments and measurements. Please note that a process model if replaced by actual experimental observations, it will cause us huge amount of money as well as it will be extremely time consuming step. So, we need a mathematical representation of the real process.

So, we will save money we will save time and also it will be safe there would not be any hazard to perform such computer experiments. But it may be unsafe to perform such experiments in real life, because you may not try you may try certain operating conditions which can lead to some disruptions or can cause potential problems in the plant. So, we heavily depend on a simple, but reasonably accurate mathematical representation or model of the physical process.

So, that we can perform computer experiments safely, quickly and economically, but at the same time we can rely on the quality of the optimal solution. Now, let us talk about various classification of process models. Process models are broadly categorized into two types, models based on physical theory, we call them theoretical models. There we make use of physical and chemical laws theoretical models are also known as first principle based models. The other type of models are models based on strictly empirical descriptions, they are data based models also known as black box models.

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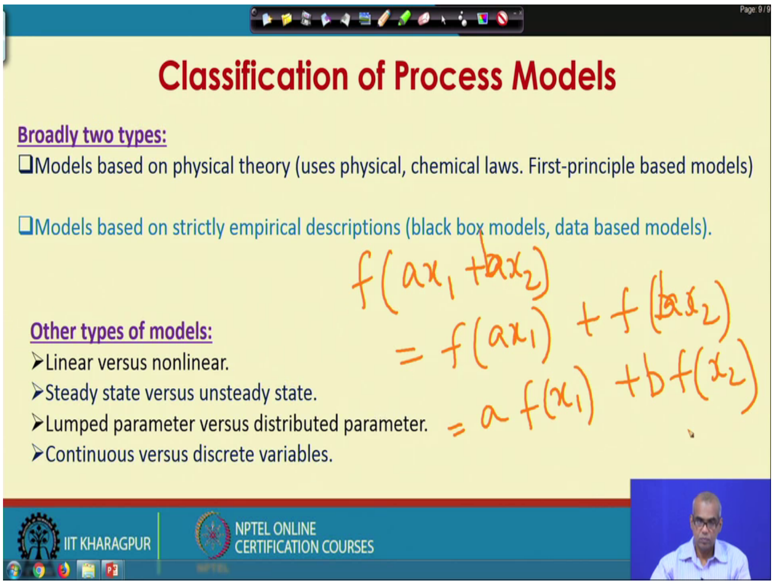

So, theoretical models and empirical models; Theoretical models are based on physical and chemical laws such as mass balance equations, energy balance equation, momentum balance equations, then various constitutive relationships such as that comes from thermodynamic relationships, kinetic relationships so on and so forth.

Other types of models are linear versus non-linear, steady state versus unsteady state, lumped parameter versus distributed parameter, continuous versus discrete variables. Let us first briefly talk about linear models versus non-linear models. In linear models all the equations are linear, in non-linear models non-linear equations are present.

So, linear models which consist of linear equations have interesting property that is of principle of super position. So, what it means is f of ax 1 plus ax 2 will be f of ax 1 plus f of ax 2. This is the principle of super position. In fact, you can also write as you can also consider this as b where a and b are constants. For non-linear models such principle of super position does not hold true. Next steady state versus unsteady state, steady state means time in variant; that means, the states of the system are time in variant or stationary.

So, steady state models represents a process where the state of the systems; that means, the variables that describe the state of the system are not changing with time. They are stationary or also known as time in variant. For unsteady state the state of the system are not constant with time they are changing with time, they are dynamic in nature. So, they are transient a CSTR continuous start tank reactor will operate under steady state, a batch reactor operates under unsteady state, continuous distillation column will operate as steady state, a batch distillation column will operate as unsteady state. Semi batch reactors or fed batch fomenters are all unsteady state operations.

Next lumped parameter versus distributed parameter models; lumped parameter models do not consider the special variation of the state or property of the system. Whereas, distributed parameter models consider the variation of the state or properties of the system in space. Consider the temperature distribution space lab the temperature changes with time as well as space. So, if you consider 1-dimensional heat conduction in it is lab the temperature distribution function is basically a function of time and space coordinate here x, if I say only that 1-dimensional heat conduction in x direction.

So, temperature t is a function x and t, so temperature is distributed in space. So, the model or mathematical expression that describes this temperature will be a partial differential equation. If I make use of a lumped parameter model for the temperature distribution, I basically assume the temperature only changes with time; the temperature does not change with space or temperature is not a function of x. So, the temperature is uniform throughout the system.

So, the equation now will not be a partial differential equation it will be in an ordinary differential equation. Sometimes lumping is possible and that reduces the complexity of the model, but every time lumping may not be possible and we must consider the distributed parameter model. Finally, continuous versus discrete models or continuous versus discrete variables, some variables or decision variables or the stead variables can take any real value. So, they are continuous.

In some models these variables are restricted to take only certain discrete values, let us say some integers values only. For example, let us say you are optimizing the design of a distillation column, number of plates or trays has to be an integer value. Similarly, in a shell and tube heat exchanger number of tubes must be an integer value, so these are discrete variables. Now, let us take examples of theoretical models and empirical model.

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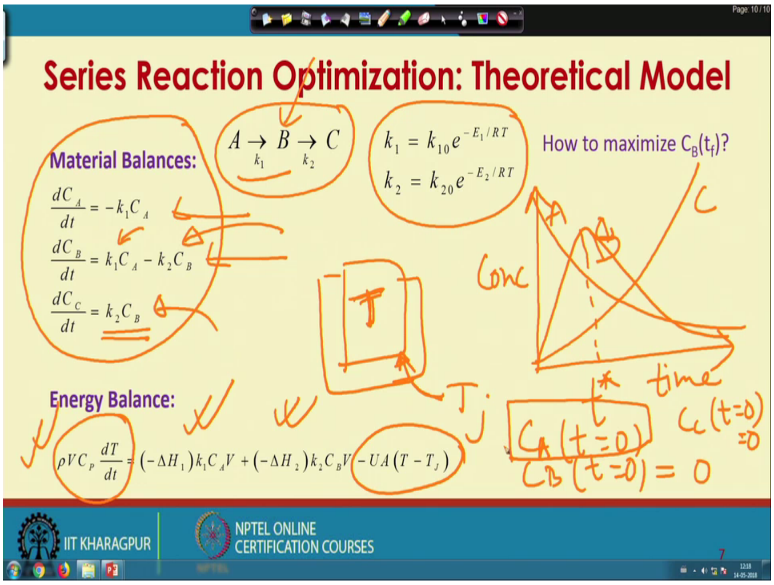

Here we consider the optimization of a series reaction which is A goes to B, B goes to C reaction that constants are given. So, these are kinetic expressions so these are the constitutive relations that we discussed previously. Now, a series reaction takes place in a reactor I want to find out the maximize, I want to find out the maximum, quantity of B. Since, it is the series reaction if the batch time is very small very less amount of B will be formed and in the batch time is more instead of more of B more of C will be formed because lot of B will get converted to C.

In fact, if you plot then concentration versus time you can intuitively feel that the concentration of A will go down with time, concentration of C will increase with time, but concentration of B will increase and then decrease. So, this is the time at which cons at which this is B. So, this is the time at which the concentration of B will be maximum, so to express this mathematically we need to write the mass balance equations for each of these components.

So, the first equation tells you the rate of change of concentration of A, so that is equal to minus k 1 into C A because due to chemical reaction A is getting converted to B. Rate of change of B which is given by d C B d t is equal to the formation of B minus decrease of B due to formation of C. Similarly the rate of change of C comes from k 2 into C B, B is only getting converted to C. If it is exothermic reaction then you have this reactor and around the reactor you have a cooling jacket. So, this jacket temperature is T j and the reactor temperature is T.

So, you have write down and energy balance equation, so this is the rate of change of temperature within the reactor which is related to the energy input due to formation, due to reaction A to B. Energy input due to reaction B to C and energy out due to heat exchange between the reactor fluid temperature T and the cooling water in the jacket whose temperature is T j. So, solutions of this equation will give me how concentration of A, concentration of B, concentration of C changes with time of course, we need the initial values.

So, we need C A at t equal to 0, C B at t equal to 0, and C C at t equal to 0. Note that C B at t equal to 0 is 0, C C at t equal to 0 is also 0. We start only with C A, so amount of C A should be specified.

So, this is theoretical model where you write mass balance equation, energy balance equation, constitutive relations to build the model. Empirical models are purely database models, what you see here is a relationship between input variable x with response y and I have the data 1 data 2 and the data 3. So, the question I ask is can I feed a linear equation through this data.

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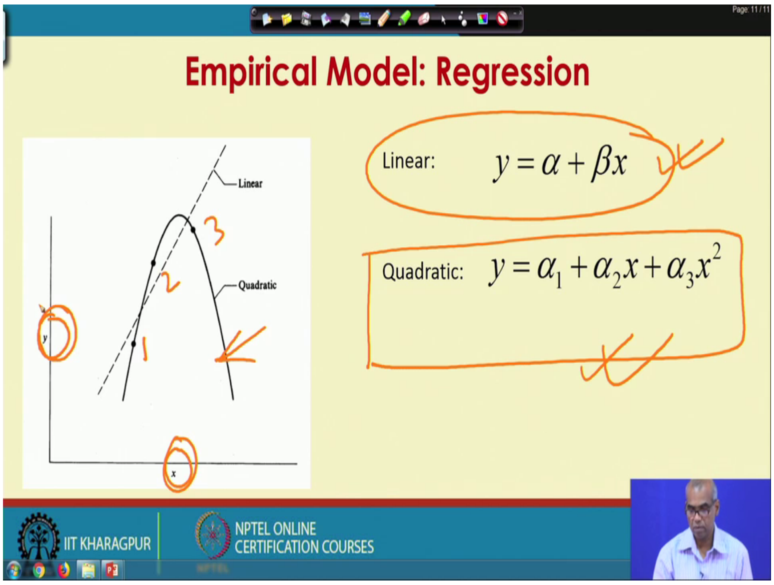

So, that these data or behaviour that exist relationship that exist between this data will be represented by this model; You see the linear fit is not very very good, but we have 3 points we can treat a quadratic equation exactly. So, this is that quadratic fit see the quadratic curve exactly passes through this point. So, this becomes a better model that represents the relationship between this input variable and the response variable. Another database models that is commonly used this days is known as neural network model.

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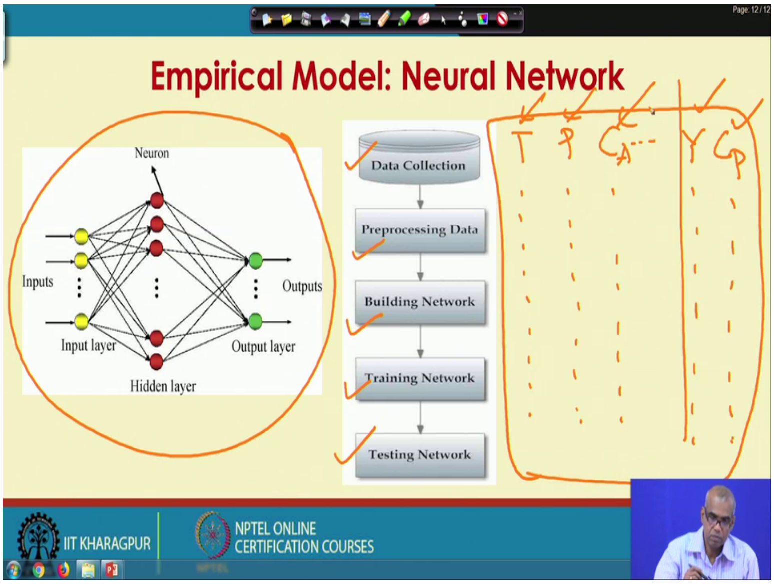

So, neural network model is also database models such as regression models. So, if we have the data large amount of data for a process, we can build a neural network to describe the relationship between input and output. Let us say you have a chemical reactor where I have this data for various temperature, pressure concentration of species etcetera and then I have let us say the yield I have the out concentration of the product etcetera.

So, we have large amount of data that I have obtained during experiments and then I use this data to build a neural network model, which involves the data collection then pre-processing the data, then building the network, then training the network which means that during the training of this network there are certain parameters within this neural network which will be adjusted. So, that during testing the neural network can predict what will be y and what will be the product concentration given any temperature pressure or these input variables.

You can learn more about neural network elsewhere, but it will be sufficient for the purpose of this course to understand the neural network is a data based model which you can build if you have good amount of data for the process. So, it is also a black box model. During training the neural network parameters will be adjusted and the neural network then can be used as a predictive tool that will give you the responses for given set up inputs.

Next let us talk about degrees of freedom analysis. The degrees of freedom analysis gives us the number of decision variables that can be changed during optimization process to obtain the optimal solution. Degrees of freedom is expressed as number of variables minus number of linearly independent equation.

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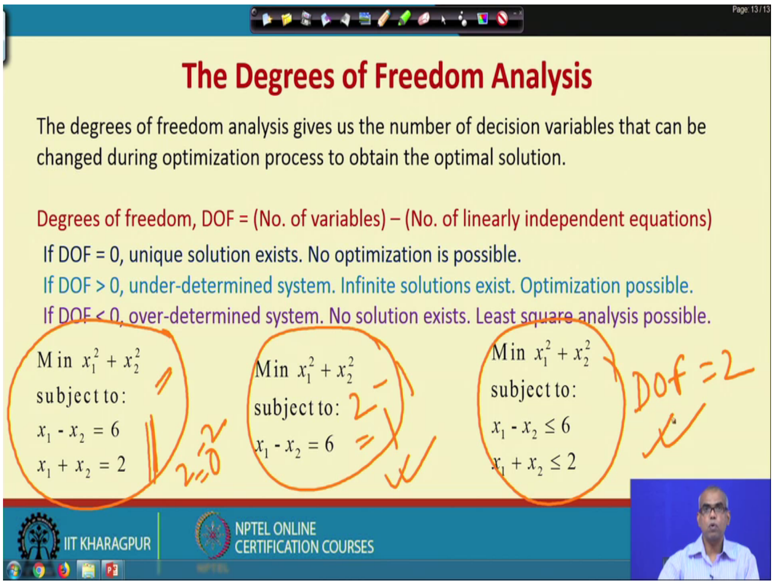

I repeat degrees of freedom equal to number of variables minus number of linearly independent equations. If degrees of freedom equal to 0 unique solution exist, no optimization is possible. Degrees of freedom greater than 0 that means, the system is under determined, in principle infinite number of solutions exist and optimization is possible because you can now choose the better solution or the best solution among alternatives. If degrees of freedom is less than 0, the system is over determined, no solution exist least square analysis is possible.

Let us look at this expression we want to minimize x 1 square plus x 2 square subject to 2 equations which are x 1 minus x 2 equal to 6 x 1 plus x 2 equal to 2. You have 2 variables, 2 equations degrees of freedom equal to 0. In fact, you can easily find out the unique solution that will exist by solving these 2 equations. Here you have 2 variables 1 equation so, degrees of freedom equal to 1 and optimization is possible. Here optimization is not possible, here optimization is possible, here you have degrees of freedom equal to 2 and optimization is possible.

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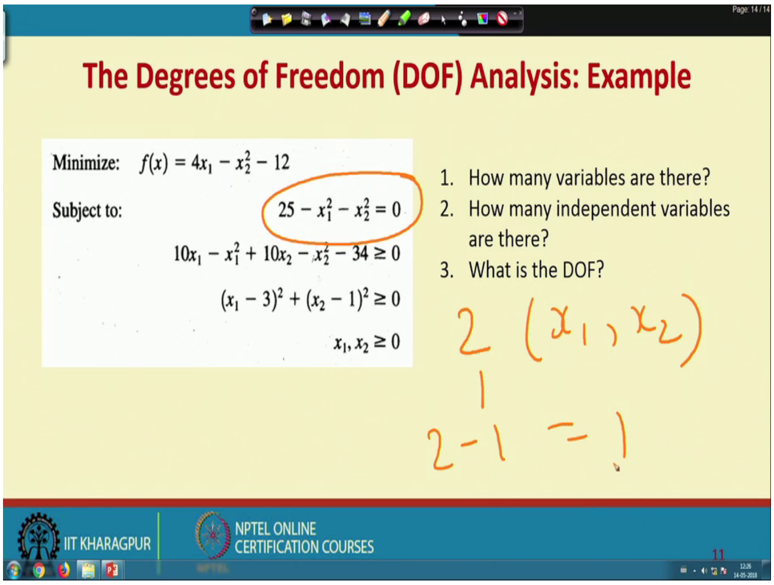

Let us look at this equation quickly, so you have an objective function which needs to be minimized, objective function as 2 variables. There is 1 equality constants, 2 inequality constants and non-negativity constants x 1 and x 2 greater or equal to 0.

So, how many variables are there variables are 2, x 1 and x 2, how many independent variables are there look at this equation; this equation can be used to express x 1 in terms of x 2 or x 2 in terms of x 1.

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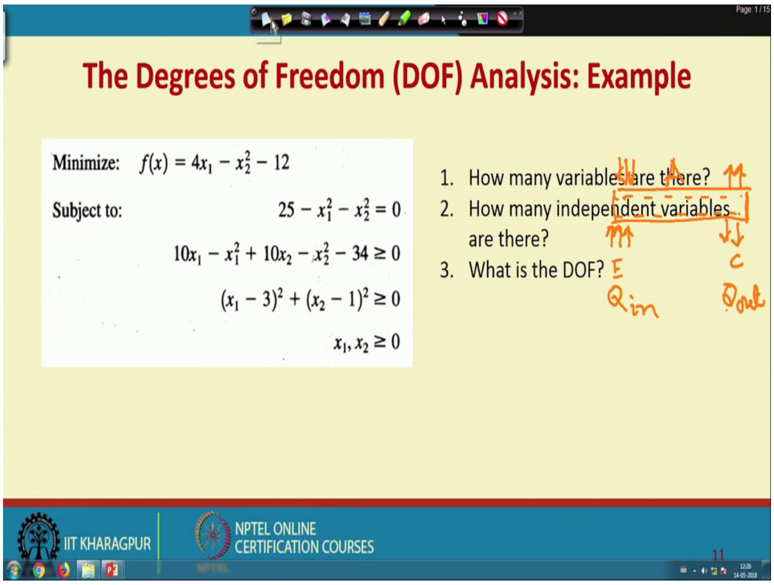

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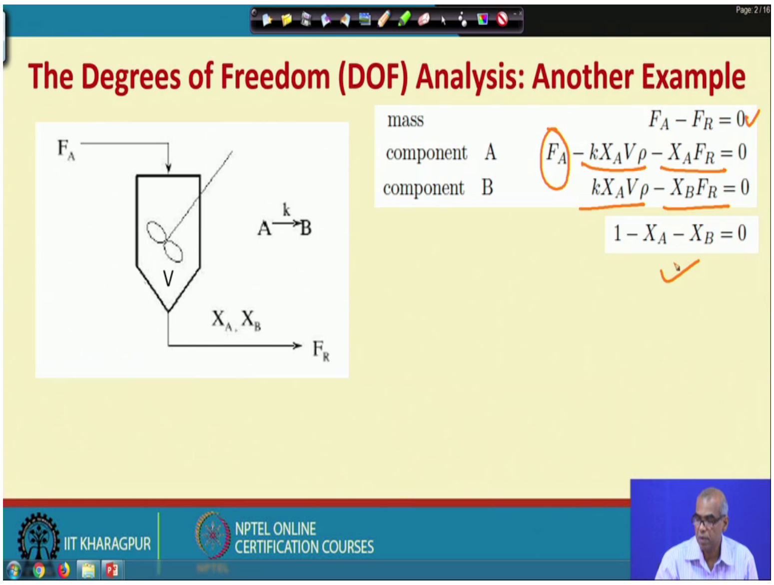

So, number of independent variable is 1, so degree of freedom is 2 minus 1 equal to 1. Final state this example p or a enters to this reactor with volume V, a reaction takes place A to B reaction at constant is k and the outlet stream the flow rate is F R, unit is mass per time and let us say the mole fractions are of A and B are X A and X B in the outlet stream.

So, the mass balance equation that will write is F A equal to F R; let us consider steady state operations or F A minus F R equal to 0. Component balance equation this is the amount F A they comes in, these due to change of A to B and these goes out with the outlet stream. Similarly the component balance B this is due to formation of B from A and this goes out with the outlet stream.

So, you can write down 1 mass balance equation 2 component balance equation, we can still write 1 more equation which is sum of all mole fractions will be equal to 1. So, X A plus X B equal to 1 or 1 minus X A minus X B equal to 0.

So, the question we ask now is if we specify F A V density of the reactor liquid inside the reactor and reaction rate constant k, we have 3 variables X A, X B and F R and we have 4 equations so, 3 variables 4 equations. What is the degree of freedom? Before that we need to ask ourselves are all the equations linearly dependent.

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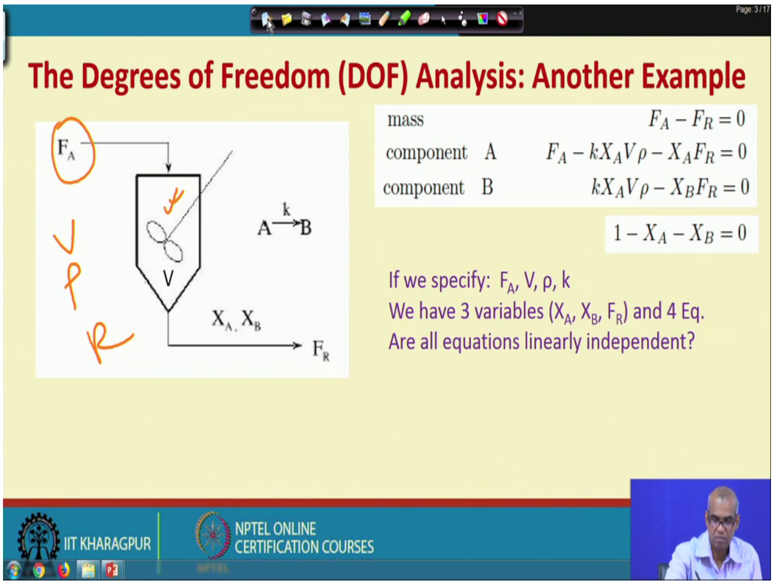

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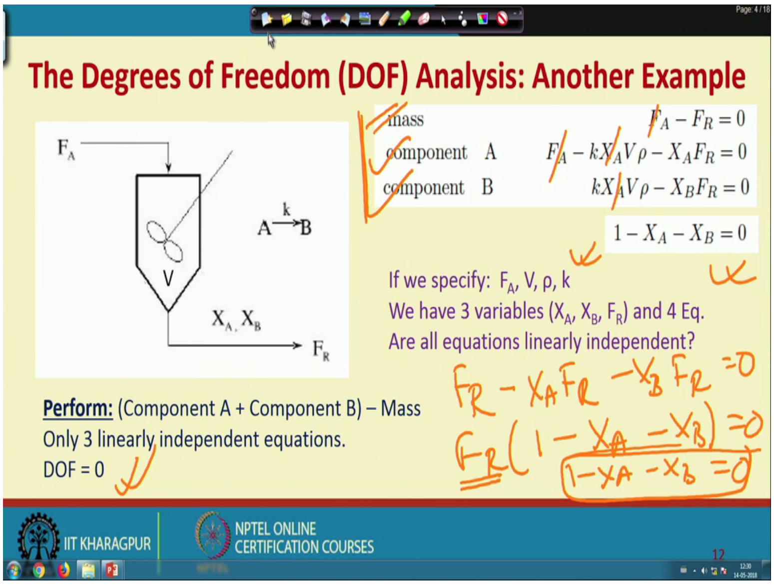

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In fact, they are not if you perform component A plus component B and then subtract that sum from this F A minus F R. So, you do component you add component A, you add these 2 equations and then subtract that from this equation; what we will get is F R because this and this will get cancel, this and this will get cancel; you will get F R minus X A F R minus X B F R equal to 0.

So, F R 1 minus X A minus X B equal to 0. Since, F R cannot be 0 1 minus X A minus X B equal to 0. So, this is the same equation. So, all this 4 equations are not linearly independent you have to drop 1 equation because from these 3 equations itself you get this equation.

So, if I drop this equation, then I have 3 variables X A, X B, F R and 3 equations my degrees of freedom is 0. Now, instead of fixing F A; if I say that F A is a decision variable that needs to be found out. So, now, I have 4 variables X A, X B, F A, F R; 4 variables 3 equations I will have degrees of freedom 1 and optimization is possible.

So, with this would like to stop here.