Optimization in Chemical Engineering
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Lecture - 07
Optimization Problem Formulation (Contd.)

Welcome to lecture 7. In this week we are talking about Optimization Problem Formulations. In the previous lecture we have talked about process models that had used for optimizations what are different types of models, classification of models and we also talked about degrees of freedom analysis. So, now onwards we will talk about formulations of optimization problems.

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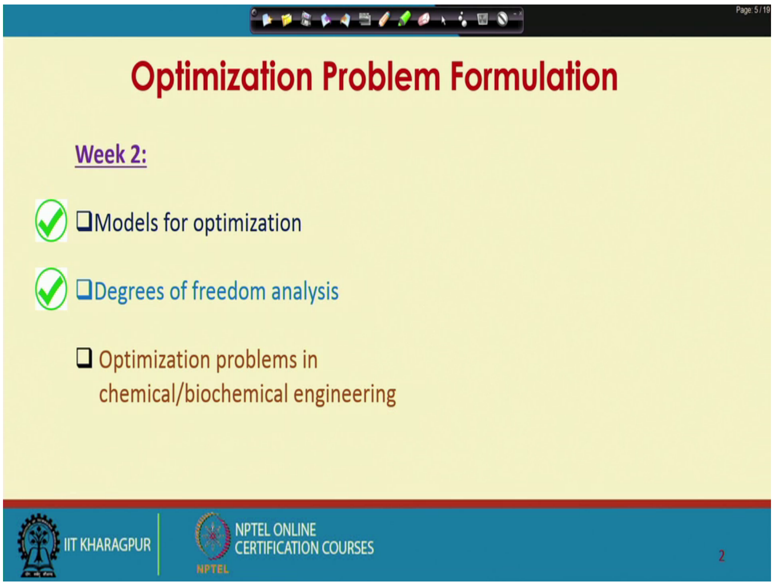

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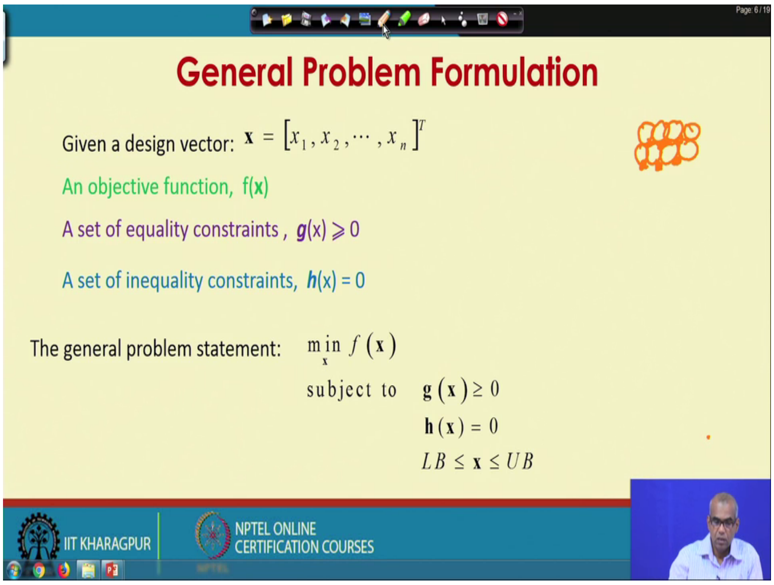

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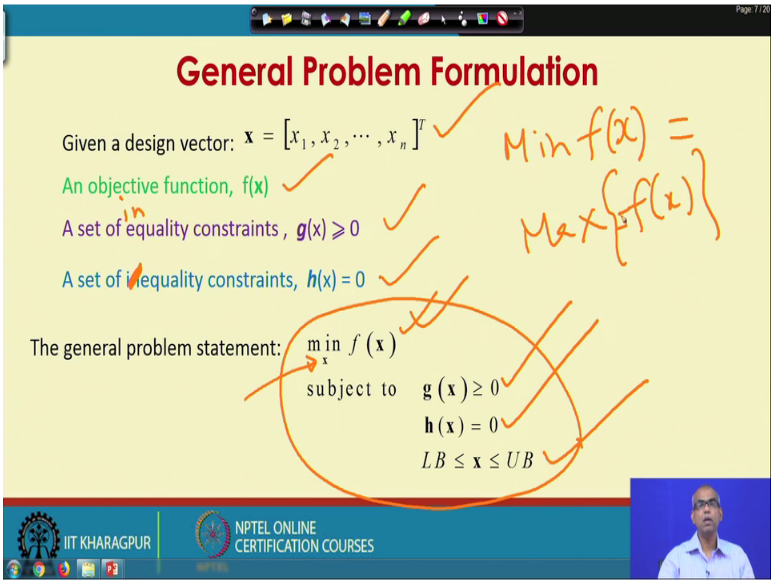

So, models for optimization and degrees of freedom analysis we have seen let us talk about optimization problems in chemical and biochemical engineering. A general problem formulation is shown here. Given, a decision variable vector or design vector x 1 x 2 up to x n; given an objective function f x, given a set of equal set of inequality constant this is inequality and this is equality, g x greater equal to 0, and set of equality constant h x equal to 0, the general problem statement is expressed as this. So you minimise the objective function f x by finding out the decision variables such that the solution obeys the inequality constant, it obeys equality constant, as well as bounds that exist on the decision variables.

So, the general problem statement or mathematical problem statement in words becomes, find out the set of decision variables that minimises an objective function which satisfy inequality constants, equality constants and bounds that exist on the decision variables. Note that, although we have written the objective function as the minimization problem, we can also write without loss of any generalisation as maximization problem. Because, minimisation of f x is same as maximisation of minus f x. So, minimisation of f x and maximization of minus f x are same.

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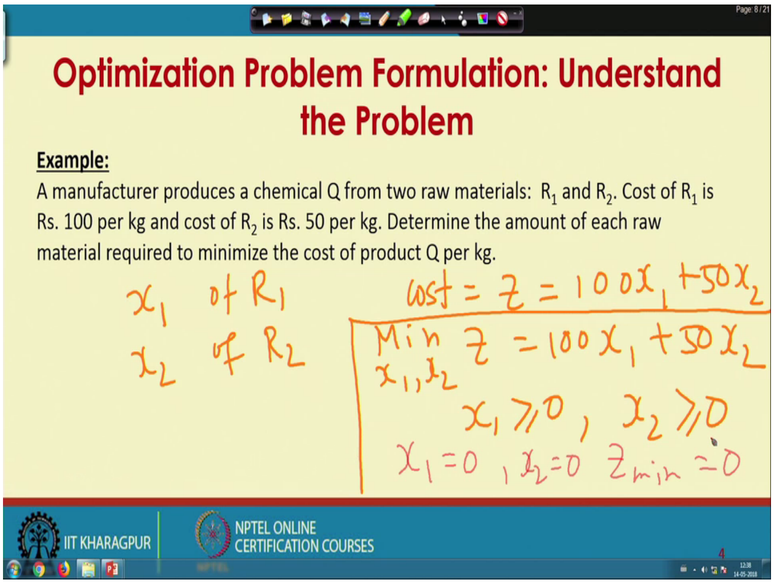

Now, to introduce the optimization problem formulation let us first consider a very very simple example. By this example will help us to understand the fact that we must have insight about the problem we are trying to work with. The problem is as follows: a manufacturer produces a chemical Q from two raw materials R 1 and R 2. The cost of R 1 is rupees 100 per kg and cost of R 2 is rupees 50 per kg. We need to determine the amount of each raw material required to minimise the cost of product Q per kg.

So, manufacturer produces a chemical Q from two raw materials R 1 and R 2 cost of R 1 is 100 per kg and cost of R 2 is rupees 50 per kg. We have to determine the amount of each raw material required to minimise the cost of product Q per kg. So, let us consider that x 1 amount of R 1 is required, and x 2 of R 2 is required to produce 1 kg of Q. R 1 is rupees 100 per kg and R 2 is rupees 50 per kg.

so the cost of x 1 and x 2, if i say that Z, Z will be 100 into x 1 plus 50 into x 2. So I want to minimise this Z, so my optimisation problem formulation will be minimisation by finding out x 2 and x 1 Z equal to 100 x 1 plus 100 x 2. X 1 and x 2 represents the amount of raw material R 1, and amount of raw materials R 2, so non negativity constants must be imposed on x 1 and x 2, so x 1 greater equal to 0 x 2 greater or equal to 0.

So this becomes the problem formulation. What is the solution to this problem? So the mathematical solution to this problem is x 1 equal to 0, x 2 equal to 0 so that Z minimum is equal to 0. Well, this is a true mathematical solution, but this is not a practical solution. So, there was something wrong in our problem formulation or there was problem in our understanding or we did not have the complete information about the problem.

So, you did not have complete information about the problem because we do not know if there is any minimum amount of product Q that must be produced. That means, a minimum amount of demand on Q is not expressed. If we do not have such a restriction that we must produce a some certain amount of Q, minimum amount of product Q, obviously the solution will be you don not produce anything, so you not have to, so cost of production will be minimum that is 0.

So, insufficient information about the problem as late to the mathematically correct solution but practically an useless solution, because to make profit you must produce the chemical. So, it is important that we have insights into the problem, so the information such as the demand of Q should be specified. So, that you know that minimum this much amount of Q has to be produce, perhaps stoichiometry is required how much of x R 1 how much of work to will react together to make the product Q. That means, the kinetic informations, stoichiometric informations maybe important.

So, again we come back to what we learned in our previous lecture that accurate mathematical description of the problem is required for useful optimisation.

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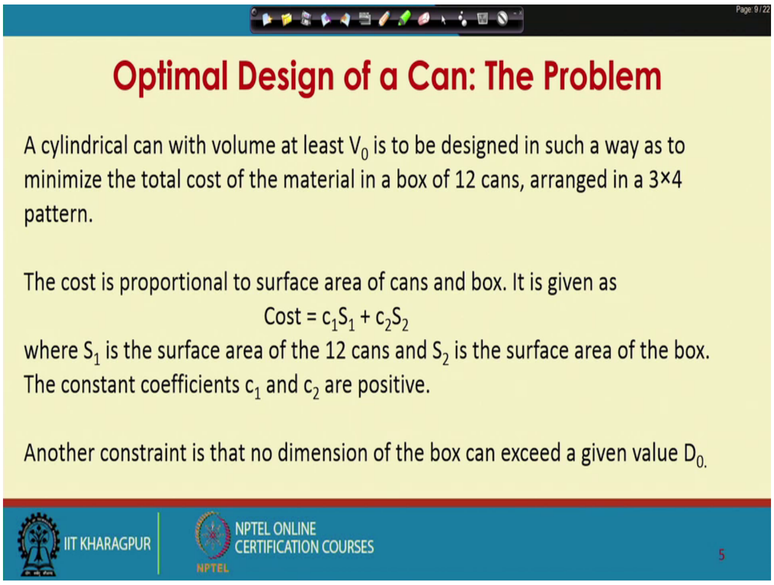

Now, let us consider a simple design problem we were talking about optimal design of a can the problem is as follows a cylindrical can with volume at least V 0 is to be designed in such a way as to minimise the total cost of the material in a box of 12 cans arranged in a 3 by four pattern. So, a cylindrical can with volume at least V 0; that means, the volume of the can must be at least V 0 problem should be greater or equal to V 0. So, these are the words we must carefully watch at least V 0 means the volume must be greater or equal to V 0.

So, cylindrical can with volume at least V 0 is to be designed in such a way as to minimise the total cost of the material in a box of 12 cans arrange in a 3 by 4 pattern. So, you will have a box of 12 cans and the total cost of the material must be minimised. So, what is information about the cost that is available the cost is proportional to surface area of cans in the box. So, that is reasonable more the surface area more amount of may be metal sheet is required to make the cans.

So, the cost is proportional to surface area of cans and surface area of the box and it is given as cost equal to c 1 S 1 plus c 2 S 2, where S 1 is the surface area of the 12 cans and S 2 is the surface area of the box the constant coefficients c 1 and c 2 are positive there is another constant which says no dimension of the box can exceed a given value D 0. So, how do I formulate this optimization problem first let us choose the design variables or decision variables I have to design suitable cans.

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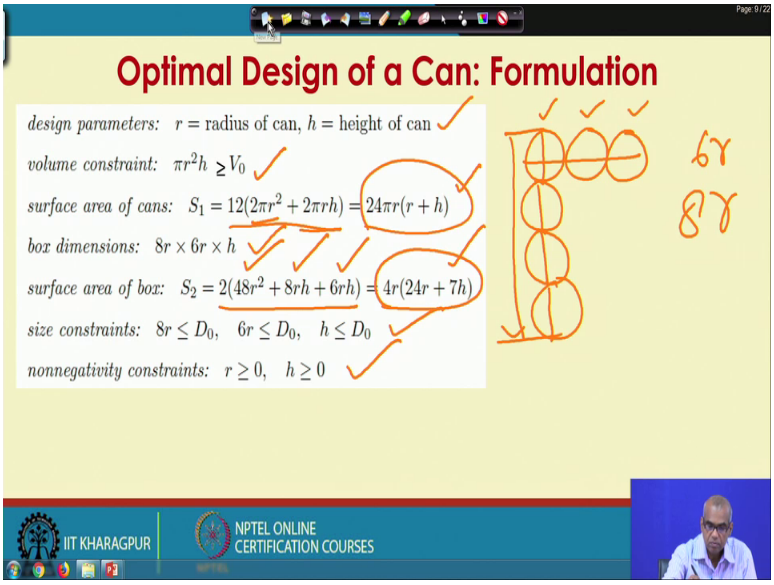

So, the natural decision variables are radius of can and height of can, so let us consider r equal to radius of can, h equal to height of can, the can must have volume greater or equal to V 0. So, the volume constant can be written as phi r square h is greater or equal to V 0, each can must have at least volume V 0. So, now let us compute surface area of can because that is required to find out that cost. So, each can has 2 surfaces at the top and bottom.

So, pi r square plus pi r square is 2 pi r square, so 2 pi r square is the surface area for the bottom and the top then the curve surface area is 2 pi r h. So, each can has surface area 2 pi r square plus 2 pi r h for 12 cans you multiply this quantity by 12. So, this becomes 24 pi r into r plus h. Now, box dimension the box will have 12 cans which are arranged as 3 by 4 let us say 3 by 4. So, this will be 2 r plus 2 r plus 2 r 6 r, whereas, these will be 2 r plus 2 r plus 2 r plus 2 r 8 r and then height h.

So, the box dimension is 8 r by 6 r by h, so surface area of the box will be how do you calculate. So, the box has dimension 8 r by 6 r by h. So, we have 2 surface areas with 8 r by 6 r dimensions. So, 48 r square 2 surface areas of 48 r square then there will be 2 surfaces with 8 r by h. So, that is gives you 8 r h for each surface and then there are 2 surfaces with 6 r and h, so each has 6 r h surface area. So, total surface area of the box is this which can be rearranged as 4 r into 24 r plus 7 h.

So, the cost can be computed as c 1 into this plus c 2 into this, there was a size constant that no dimension of the box will exceed the value D 0. So, 8 r 6 r h are the 3 dimensions they all must be less or equal to D 0 of course, there will be non negativity constants on r and h. So, the cost function can be computed easily now. So, the formal formulation can be written as minimum minimise the cost function which is written here.

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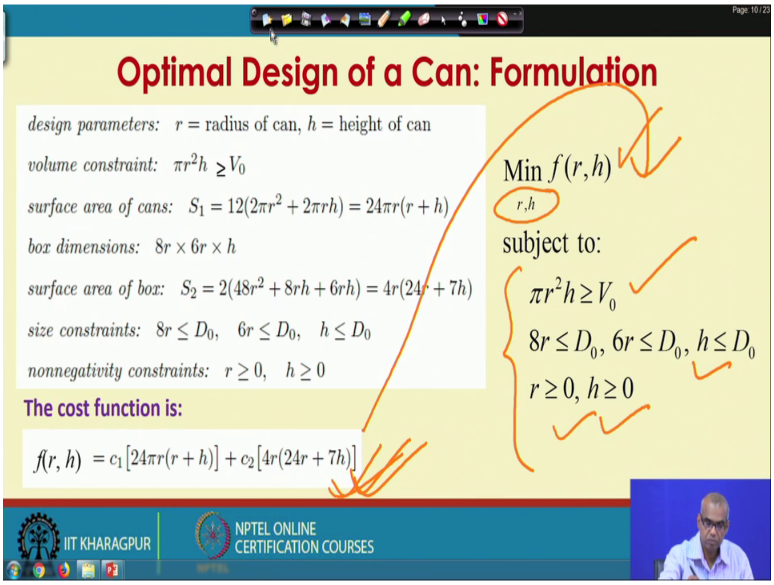

So, the cost function you can write here you have to find out r and h to minimise this cost function and the solution must satisfy these constants pi r square h greater or equal to V 0 which is the volume constant. And then the size constants 8 r less or equal to D 0 6 r less or equal to D 0 h less or equal to D 0 and non negativity constant r greater or equal to 0 h greater or equal to 0. So, this is the problem formulation for the optimal design of the can.

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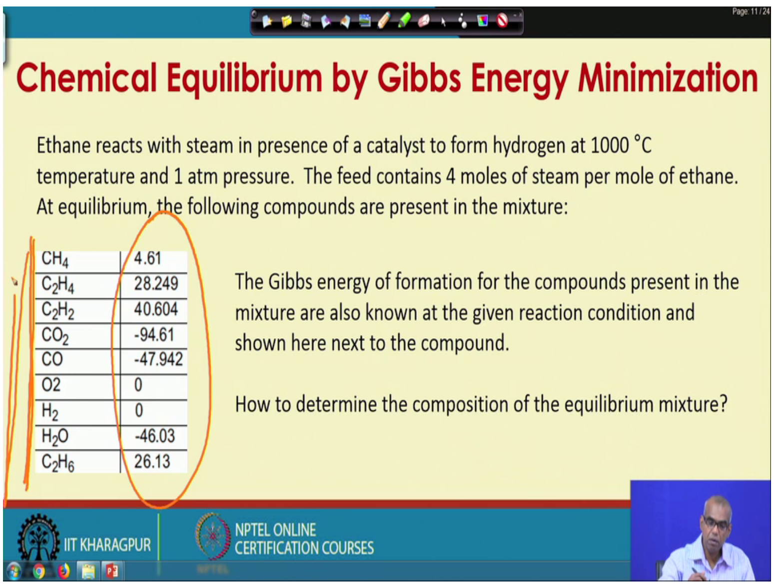

Next we will talk about another optimisation problem formulation where we find out the composition of a mixture at equilibrium using Gibbs energy minimisation. Let us consider the problem as follows ethane reacts with steam in presence of a catalyst to form hydrogen at 1000 degree Celsius temperature and 1 atmosphere pressure. The feed contains 4 moles of steam per mole of ethane at equilibrium the compounds that are present are this, CH 4, C 2 H 4, C 2 H 2, CO 2, CO, O 2, H 2, H 2 O, C 2 H 6. The Gibbs energy of formation for the compounds present in the mixture are also shown.

So, these are the Gibbs energy of formation for these compounds how do i determine the composition of the equilibrium mixture. So, ethane reacts with steam in presence of catalyst to form hydrogen at 1000 degree Celsius and 1 atmospheric pressure it in the reacts the reaction mixture also contains CH 4, C 2 H 4, C 2 H 2, CO 2, CO, O 2, H 2, H 2 O, C 2 H 6.The Gibbs energy of formation for all these compounds are known how do i determine the composition of the equilibrium mixture.

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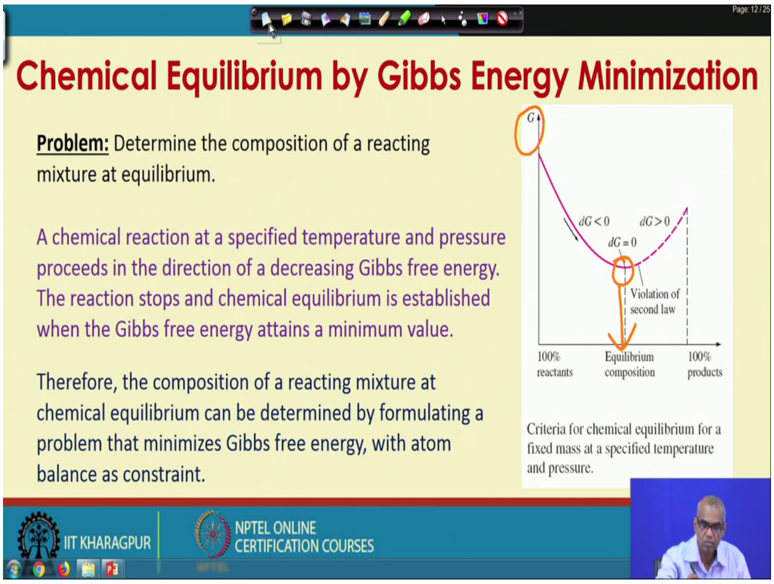

So, the problem imposes determine the composition of reacting mixture at equilibrium, a chemical reaction at a specified temperature and pressure proceeds in the direction of a decreasing Gibbs free energy. The reaction stops and chemical equilibrium is establish when the Gibbs free energy attains a minimum value. Therefore, the composition of a reacting mixture at chemical equilibrium can be determined by formulating a problem that minimises Gibbs free energy with atom balance as constants you have reactants and then products.

So, the condition is this, that the Gibbs free energy will be minimum at equilibrium, so the reacting mixture at equilibrium must satisfy the minimisation of Gibbs free energy it also satisfy the atom balance. So, atom balance will be use as a constant and the objective function will be the Gibbs free energy which will be minimised. So, the figure shows you that this is the equilibrium composition where the Gibbs free energy attains the minimum value, to formulate this optimization problem.

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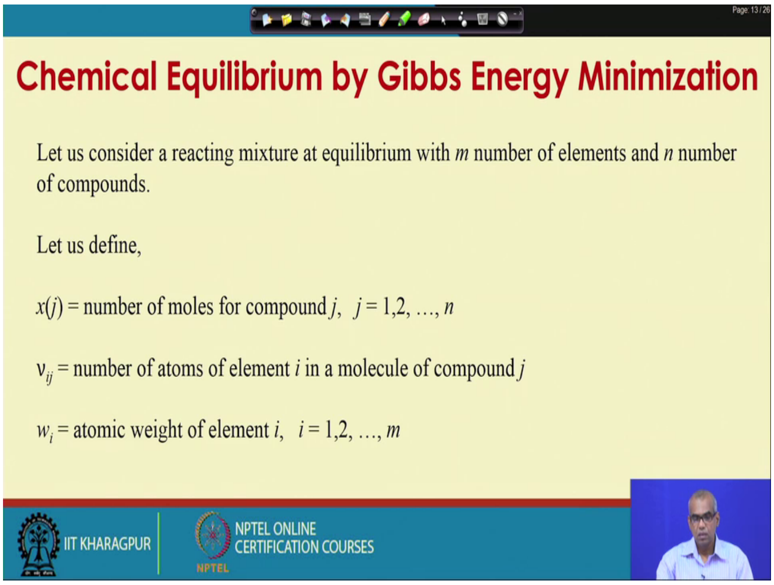

Let us consider the reacting mixture at equilibrium let us consider there are m number of elements and n number of compounds. We define xj equal to number of moles of compound j, so j varies from 1 to n n number of compounds let us consider nu ij is number of atoms of element i in a molecule of compound j. So, in a molecule of compound j there are number of atoms of element i. So, nu ij is the number of atoms of element i in a molecule of compound j and w i is the atomic weight of element i i goes from 1 to m because there are m number of elements.

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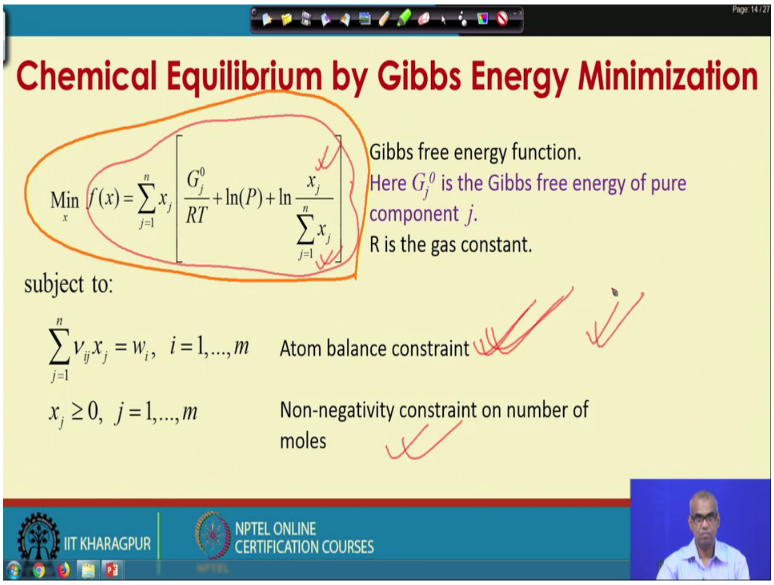

So, the Gibbs free energy function is given by this, in fact, this so sigma xj j equal to 1 to n into Gj 0 by RT plus ln P plus ln xj divided by some of all moles, here Gj 0 is the Gibbs free energy of the pure component j it was given in the problem. So, we can compute P is the pressure R is the universal gas constant. So, this objective function which represents Gibbs free energy has to be minimised. So, you find out number of moles of compound j to minimise the objective function subject to the atom balance constant.

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So, sigma j equal into n nu ij x j will be equal to w i where wi is the atomic weight of the element i. So, this atom balance constant must be satisfied and of course, non negativity constant or number of moles, so xj greater or equal to 0. So, the determination of the equilibrium mixture by minimising the Gibbs free energy can be formulated as this.

With this, we will stop lecture 7 here.