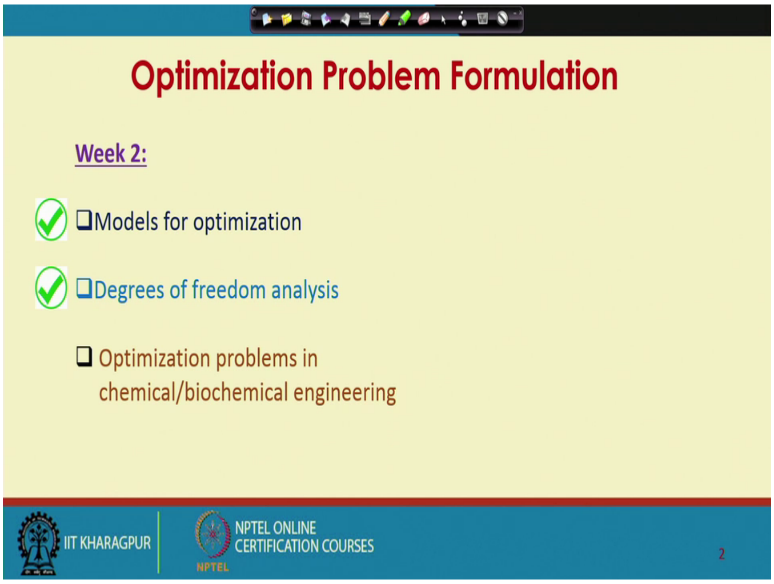
Optimization in Chemical Engineering

Prof. Debasis Sarkar
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur

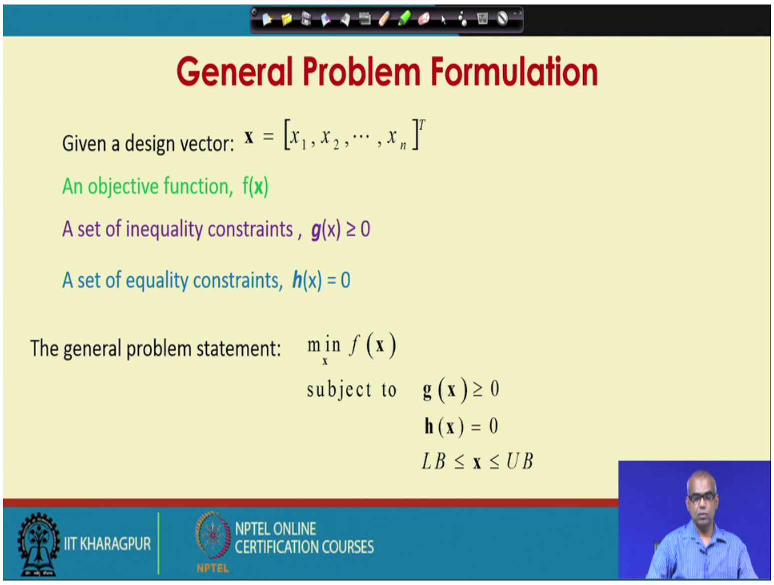
Lecture - 10
Optimization Problem Formulation

Welcome to lecture 10. So, this is the last lecture of week 2 and we will continue our discussion on Optimization Problem Formulations. So, today we will take 2 examples one from refinery blending problem and another heat exchanger optimization problem. In case of heat exchanger optimization problem we will have an economic objective function and we will conclude this lecture with a very brief discussion on net present value, which is often consider when we have economic objective functions.

(Refer Slide Time: 01:06)

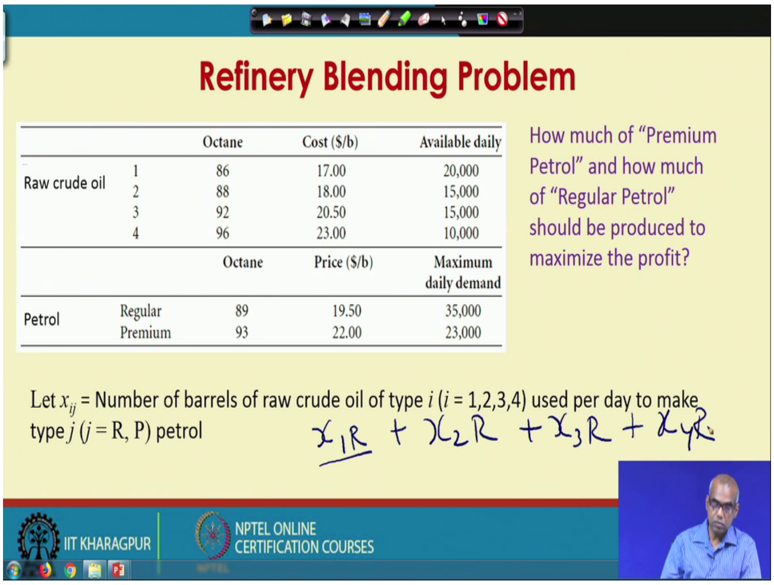


(Refer Slide Time: 01:20)



So, let us start our discussion on optimization problems in chemical biochemical engineering. So, a quick review if you have a design vector or decision vector n vector say x 1, x 2, up to x n. If you have an objective function f x, if you have a set of inequality constraint g x greater or equal to 0, if you have a set of equality constraint h x equal to 0, then the general problem statement for optimization can be written as shown. So, minimisation of f x subject to g x greater or equal to 0, h x equal to 0, x is bounded between lower bound and upper bound.

(Refer Slide Time: 02:16)



		Octane	Cost ($/b)	Available daily
Raw crude oil	1	86	17.00	20,000
	2	88	18.00	15,000
	3	92	20.50	15,000
	4	96	23.00	10,000
		Octane	Price ($/b)	Maximum daily demand
Petrol	Regular	89	19.50	35,000
	Premium	93	22.00	23,000

So, let us now talk about the refinery blending problem. The data you show the data you see is a typical data from a refinery which blends 4 different types of crude oils, to make 2 types of petrol. So, there are 4 different types of crude oils which are blended in different proportions to make regular petrol and premium petrol. The octane number of each crude oil is specified. The cost of each crude oil is specified and also the quantity available daily is available for each crude oil.

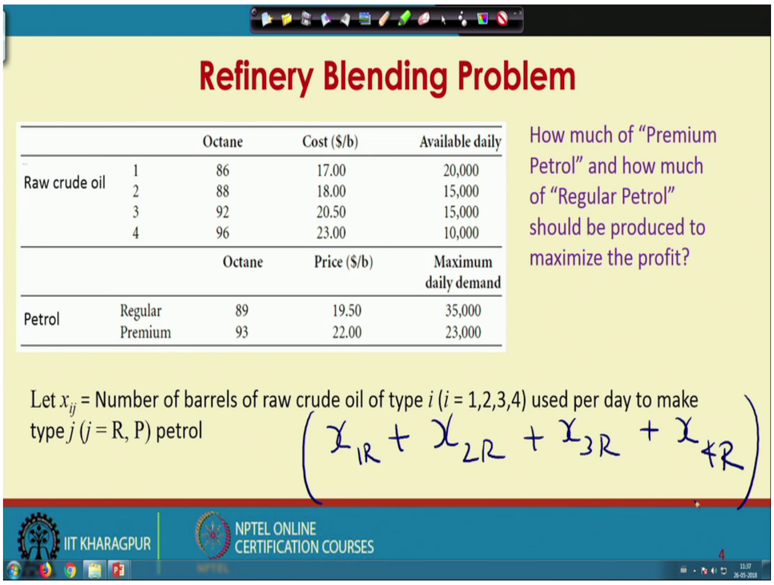
The regular petrol must have an octane number 89 or greater than that, premium petrol must have octane number 93 or higher a minimum octane number of 89 and 93 has to be maintained for regular petrol and premium petrol respectively. The selling price of regular petrol is 19.5 dollar per barrel, selling price of premium petrol is 22 dollar per barrel B is stands for barrel. Also daily maximum demand for regular petrol is 35000 barrel and premium petrol it is 23000 barrel. The crude oil availability is also given in terms of barrels.

So, given this data we need to find out how much of premium petrol and how much of regular petrol should be produced so, the profit is maximise. So the question a asked is how much of premium petrol and how much of regular petrol must be produced to maximise the profit. So, to do that we need to know how much of crude oil 1, 2, 3 and 4 should be mixed together to make regular petrol and in what quantity of crude oil 1, 2, 3, 4 must be blended to produce premium petrol.

So, if you look at this the decision variable seems to be the quantity of crude oil 1, 2, 3, and 4 to be blended to make regular petrol and quantity of crude oils 1, 2, 3, 4 to be blended to make premium petrol. So, there are 4 plus 4 8 decision variables. So, you can write using mathematical notation as let X ij with the number of barrels of raw crude oil of type a where i will vary from 1 2 3 4 four types of crudes used per day to make type j petrol for type j is either regular or premium. So, use R for regular and use the letter P for premium.

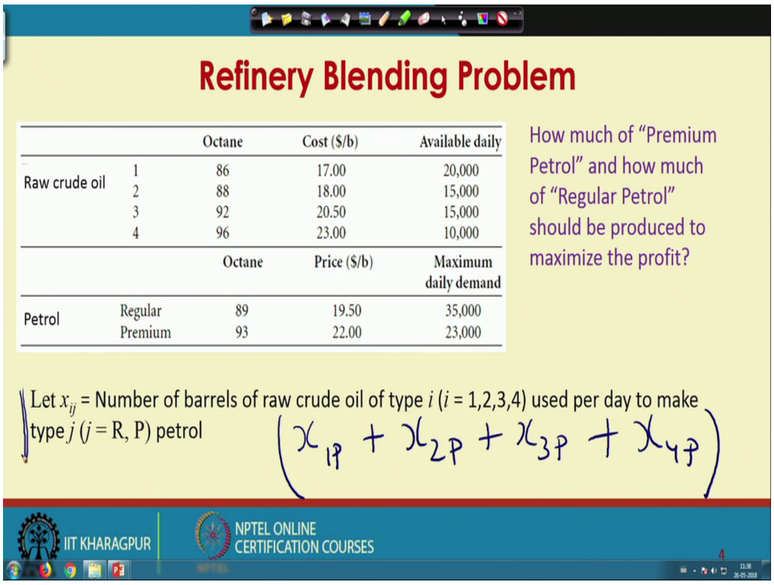
So, X ij where i goes from 1 to 4 and j goes from 1 to 2; that means, R and P are my decision variables. So, x 1R is the amount of crude oil 1, I will chose to make regular petrol. So, regular petrols will be made by mixing x 1 barrels of crude oil 1 plus x 2R barrels of crude oil 2, plus x 3R barrel of crude oil 3 and x 4R barrel of crude oil 4. These R has basically suffix so I should write like x 1R plus x 2R plus x 3R plus x 4R.

(Refer Slide Time: 08:08)

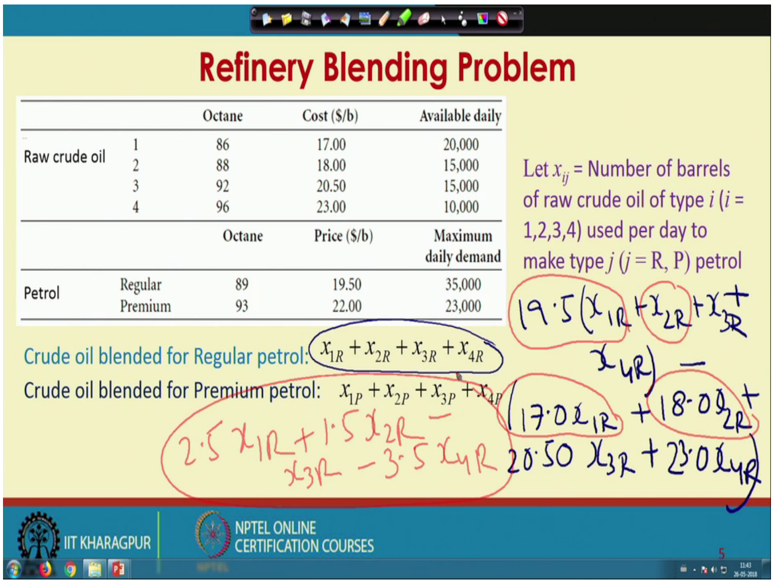


So, I will choose x 1R barrel from crude oil 1, x 2R barrel of crude oil 2, x 3R barrel of crude oil 3 and x 4R barrel of crude oil 4 and blend them to make regular petrol. So, what will be the quantity produced? The quantity produced will be x 1R plus, x 2R plus, x 3 4 R plus, x 4R barrel of regular petrol. Similarly, I will take x 1P barrel of crude oil plus x 2P barrel of crude oil 2 plus x 3 x 3P barrel of crude oil 3 plus x 4 P barrel of crude oil 4 to make premium petrol.

(Refer Slide Time: 08:56)



(Refer Slide Time: 09:50)



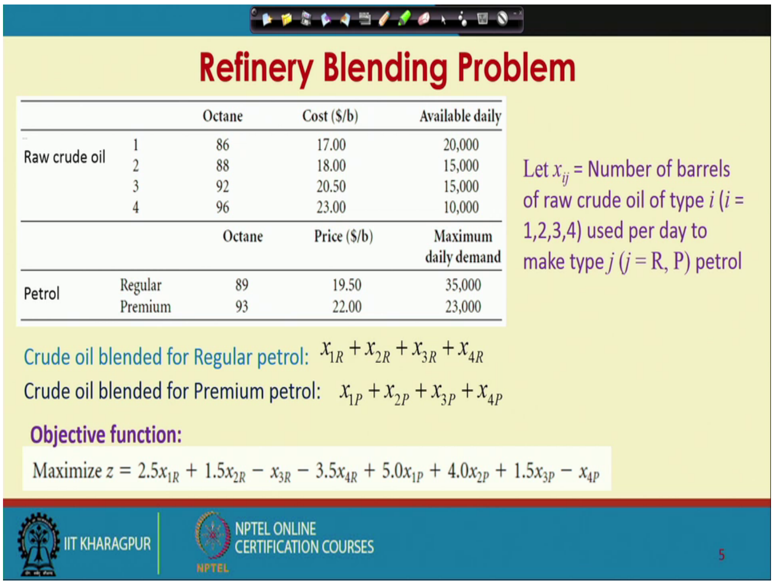
So, this is the notation we are going to use, this is what is meant by x ij i goes to 1 to 4 and j goes to R and P. So, this is the crude oil blended for regular petrol x 1 4 plus x 2 4 x 2R plus x 3 R plus x 4, similarly crude oil blended for premium petrol is x 1 P plus x 2 P plus x 3 P and x 4 P. So, the quantity produced are also these many barrels.

Now, these are the decision variables also x 1R, x 2R, x 3 R, x 4R and x 1P, x 2P, x 3P, x 4P so these are the 8 decision variables. Now I need to formulate the objective function. So, here I want to maximise the profit so the profit is selling price minus cost price. So, let us find out the profit from regular petrol and profit from premium petrol then you add these 2.

So, let us first consider regular petrol so what will be the profit for regular petrol? So, the regular petrol has a selling price of 19.5 so 19 so 19.5 into x 1R, plus x 2R plus x 3R plus x 4R. So, this is the amount I will get by selling this quantity of regular this much barrel of regular petrol and the cost will be 17 dollar per barrel of crude oil 1. So 17 one 0 x 1R for x 2R it will be 18.0 in to x 2R plus 20.50 into x 3R plus 23.0 into x 4R. So, this is the quantity this is the amount which is the selling price sorry the cost price. So, this let us put within bracket. So, we have to take the difference between the selling price and cost price.

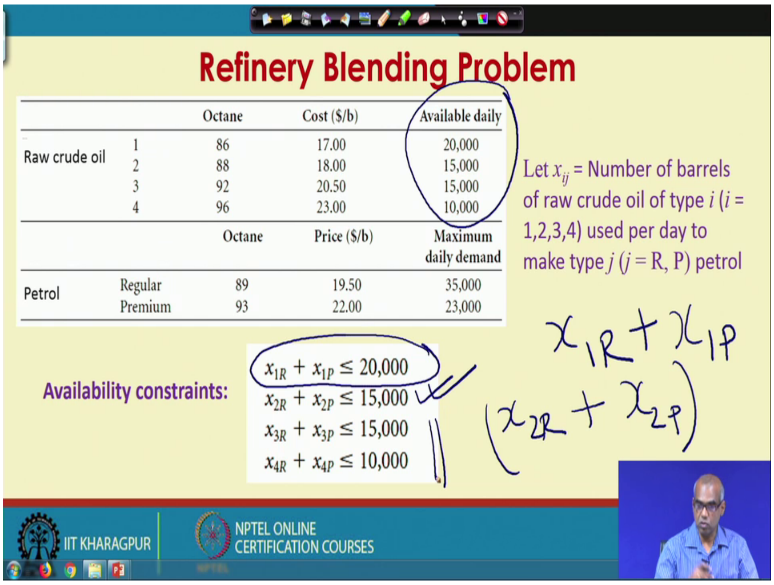
So, let us look at this 19.5 into x 1R minus 17 into x 1R, so this becomes 2.5 x 1R next 19.5 into x 2R minus 18 x 2R; that means, plus 1.5 x 2R, then 19.5 x 2 x 3 R minus 20.5 x 3R. So, we have a loss here minus 1 in to x 3R; that means x 3R then 19.5 into x 4R minus 20.3 into x 4R; that means 3.5. So, again minus 3.5 x 4 R, so this is the profit that I get from regular petrol. Similarly you have to do the same thing to obtain profit from the premium petrol and then add these 2 if you do this you will get this.

(Refer Slide Time: 14:33)



Note that we just calculated it this much, similarly you calculate it the profit that will obtain from the premium petrol you add this 2. So, this is the total profit let us call it z. So, my objective function will be maximise this z. So, I have to find out these 4, this 8 4 plus 4 8 decision variables to maximise the objective function z, which is given by this equation and this equation is nothing, but the selling price minus the cost price selling price of the regular petrol and premium petrol minus cost price of the crude oils.

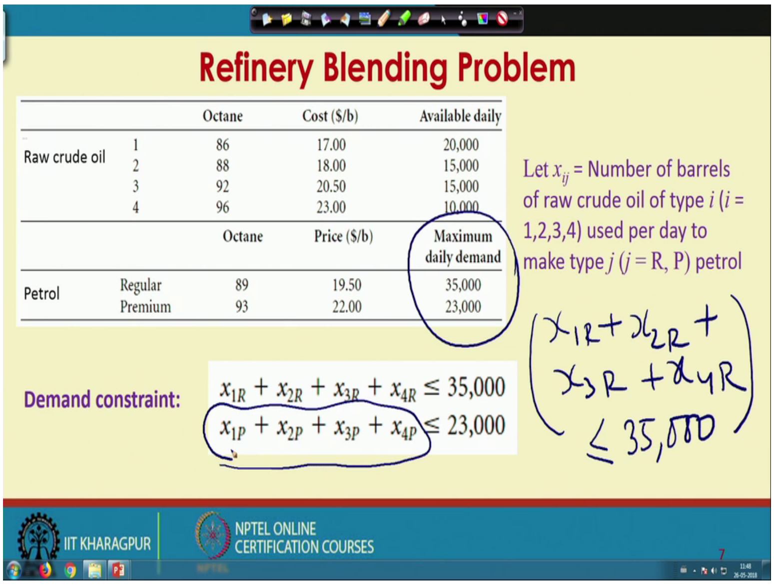
(Refer Slide Time: 15:44)



So, once I have found out the objective function, I now need to find out the constraints. What are the constraints? First consider is this that we have a constraint on daily availability of 4 crude oils for example, the crude oil 1 is available at 20000 barrel per day. So, I cannot exceed 20000 barrels of crude oil per day, similarly I cannot exceed 15000 barrel of crude oil 2 so, on and, so forth.

Now, I use x 1R of crude oil to make regular petrol and I use x 1P barrel of crude oil 1 to make premium petrol. So, the total amount of crude oil 1 I use is x 1R plus x 1P. So, x 1R plus x 1P must not exceed 20000. So, this is the constraint on crude oil 1. Similarly I use x 2R barrel of crude oil 2 to make regular petrol and x 2P barrel of crude oil 2 to make premium petrol. So, the total amount of crude oil 2 I use is x 1 2R plus x w P x 2R plus x 2 p. So, x 2R plus x 2 P must not exceed 15000, similarly you can write the other 2 constraints which are availability constraints here.

(Refer Slide Time: 17:46)

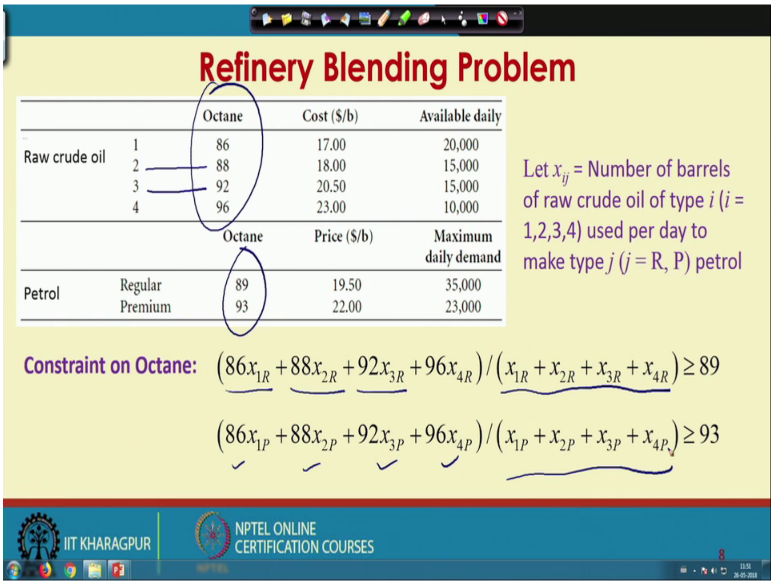


So, are there any other constraint yes we have demand constraint. The maximum daily demand for regular petrol is 35000 barrel and the maximum daily demand for premium petrol is 23000 barrel. So, it does not make sense to produce more than 35000 of regular 30000 35000 barrel of regular petrol and more than 23000 barrel of premium petrol.

So, what is the total amount of regular petrol I am making per day? X 1R plus x 2R plus x 3R plus x 4R. So, this is the total quantity of regular petrol I am using I making the blending 4 different crude oils. So, this quantity must not be greater than 35000. Similarly I am using x 1P, plus x 2P plus x 3P plus x 4P barrel of premium petrol and the maximum daily demand for premium petrol is 23000 barrels. So, x 1P plus x 2P plus x 3P plus x 4P should be less or equal to 23000 barrel. We have to take care of this inequality whether it is lesser equality or greater equality.

So, if it was told that the minimum daily demand is 35000 and minimum daily demand is 23000 then you would have used greater or equal to instead of less or equal to. So, please take care of the problem statement whether you are given minimum daily demand or maximum daily demand here we are given maximum daily demand. So, demand does not exceed 23000 barrel or 35000 barrel. So, we would not produce more than that.

(Refer Slide Time: 20:35)

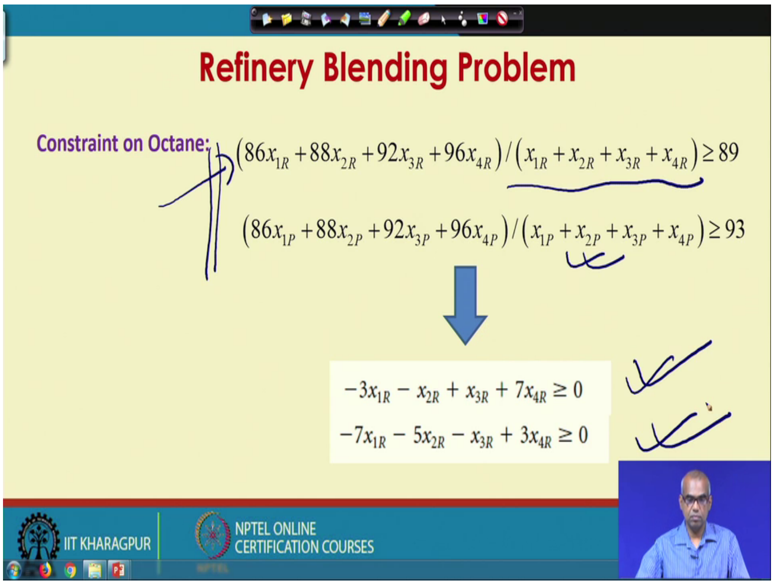


So, we talked about constraint on daily availability and constraint on maximum daily demand. Now there is one more constraint, which is constraint on octane number octane numbers of crude oil are given and octane number of regular petrol and premium petrol are specific. So, octane number of regular petrol must be at least 89. So, it should be greater or equal to 89. Similarly octane number of premium petrol should be at least 93; that means should be greater or equal to 93.

Now, I am using x 1R, x 2R, x 3R and x 4R barrels of crude oil 1 2 3 4. So, to make to find out the octane number of the blended petrol what I do is, I take the weighted average. So, crude oil 1 octane number is 86 and I am using x 1R barrel of crude oil 1. So, I write 86 into x 1R plus 88 into x 2R plus 92 into x 3R plus 96 into x 4R divided by the total number of barrels. So, that must be greater or equal to 89.

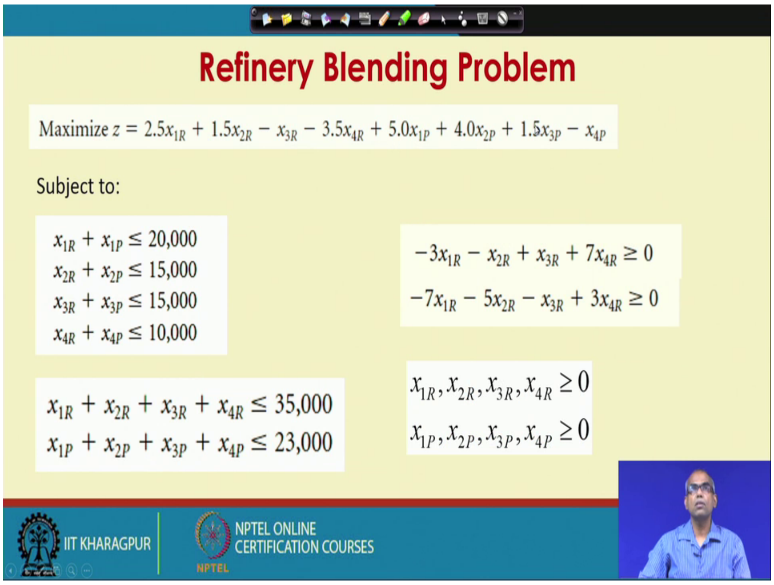
Similarly, I find out the average octane number of the blended premium petrol from the knowledge of individual octane number of the crude oils and the total quantity of the premium petrol. So, these octane number must be greater or equal to 93, see if such constraint is not there, there is no constraint on the octane number then to maximise the profit one you blend, the maximum amount of that crude oil which has minimum price, and that will be the crude oil with the rest octane number. So, the octane number must be made and that in fact, restricts the quantity of different petrols different crude oils that has to be blended appropriately.

(Refer Slide Time: 23:49)



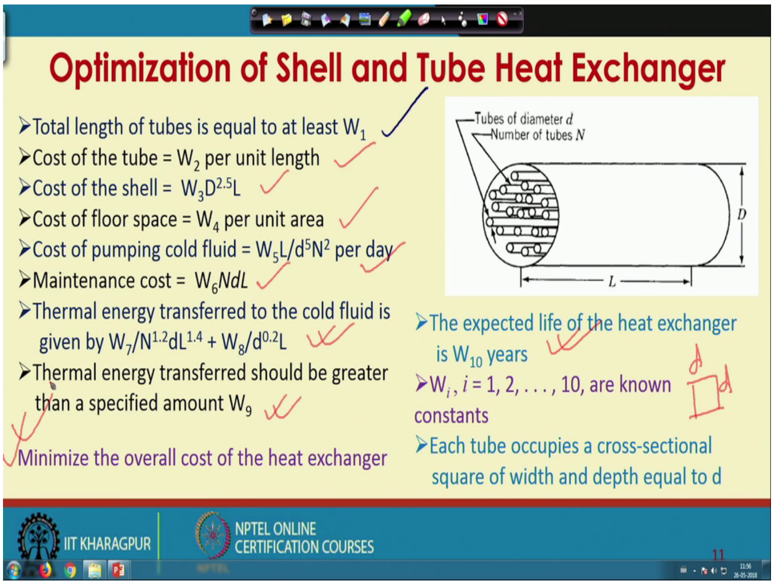
So, now these 2 constraint on the octane number can be written after rearrangement as this. What it is simple what you do is let us talk about this you multiply both sides by this and then rearrangement you will get this. Similarly you multiply both sides of this by this denominator and rearrange, and you will get this constraint. So, now, we have objective function we have all the constraints so, the refinery blending problem now can be formally stated as follows.

(Refer Slide Time: 24:28)



So, maximise date equal to this which is the objective function subject to this availability constraint, subject to these daily demand constraint, subject to this constraint on octane number and the non negativity constraint which says that x 1R, x 2R etcetera must be greater or equal to 0.

(Refer Slide Time: 25:03)

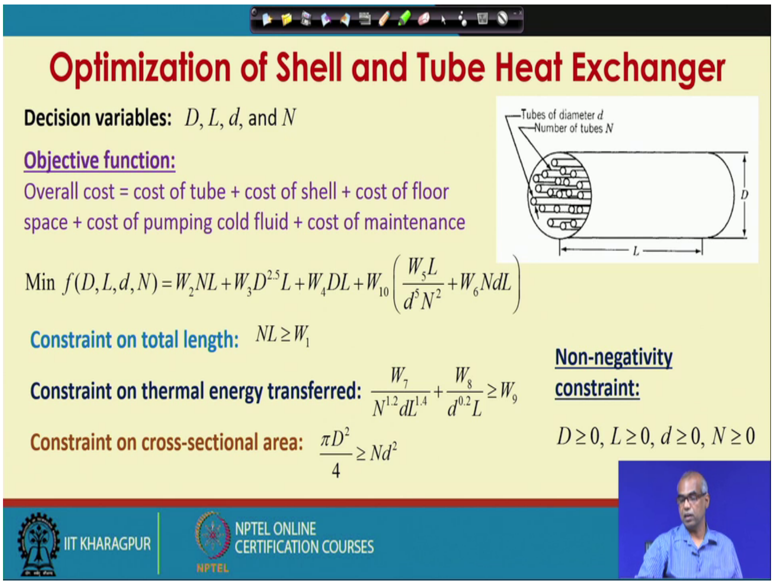


Next we briefly talk about optimization of shell and tube heat exchanger. As you see in the diagram we have a shell of length L diameter D and the error capital N number of tubes each tube has diameter small d. We want to minimise the overall cost of the heat exchanger by appropriately choosing the length of the shell L, diameter of the shell D capital D N number of tubes N and diameter of the tube small d. So, the data are given total length of the tube is equal to at least W 1 cost of the tube is W 2 per unit length, cost of the shell is W 3 into capital D to the power 2.5 in L.

Capital D is the diameter of the shell, capital L is the length of the shell, cost of the floor space W 4 per unit area cost of pumping cold fluid. W 5 into L divided by small d to the power 5 N square per day, maintenance cost is W 6 in to N into small d into L, thermal energy transferred to the cold fluid is given by this expression and thermal energy transferred should be greater than the specified amount say W 9. The expected life of the heat exchanger is W 10, years all this W 1, W 2 up to W 10 are known constants.

We also assume that each tube occupies a cross sectional square of width and depth equal to d. So, each tubes occupies an area small d square. So, we need to minimise the overall cost of the heat exchanger. So, how do I formulate the optimization problem? So, it is quite clear that the objective function will be economic in nature. So, the decision variables are capital D diameter of the shell, capital L length of the shell small d diameter of the tubes and capital N, which is the number of tubes in the shell.

(Refer Slide Time: 27:40)



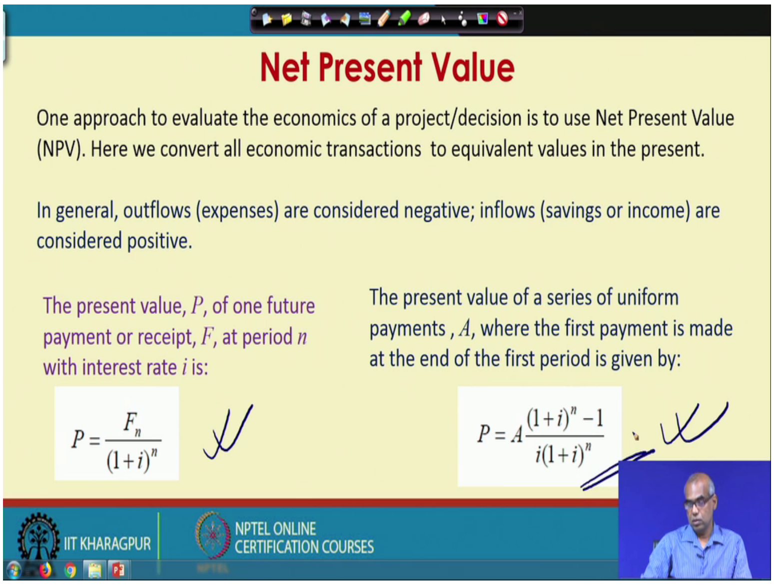
Objective function we are minimising cost. So, overall cost will be the objective function what is the overall cost? Overall cost is cost of tube plus cost of shell plus cost of floor space plus cost of pumping cold fluid plus cost of maintenance. So, the objective function is a function of 4 decision variables. The cost of tube where capital N tubes they have length L. So, the cost of tube is W 2 into NL cost of shell according to there are data given is this, cost of floor space cost of floor space is proportional to the area.

So, you need an floor area D times L capital D times capital L. So, W 4 into capital D in to capital L is the cost of floor space. Cost of pumping cold fluid and cost of maintenance is dependent on the life of the heat exchanger because it will depend on the number of days or number of years will be operating. So, this is the term if you look at the data given in the previous slide represents the cost of pumping cold fluid and this is the cost of maintenance.

Now, I multiplied by W 10 which represents the life of the heat exchanger, W 10 years you can also multiply and these are in terms of days. So, you can actually multiply by 365, even if you do not multiply the optimal values of these capital D capital L small d and capital N will not change, but this cost quantity of the cost amount will change, but the optimal solution will not change because it is getting multiplied by a constraint.

So, this total cost presence the objective function constraint. On total length each tube has length L. So, N into L must be greater or equal to W 1, constraint on thermal energy transferred must be greater or equal to specified quantity W 9, constraint on cross sectional area the shell has area pi capital D square by 4. So, that is must be enough to accommodate n number of tubes. So, each tube takes small d square cross sectional area as told in the previous slide. So, we have n cap tubes.

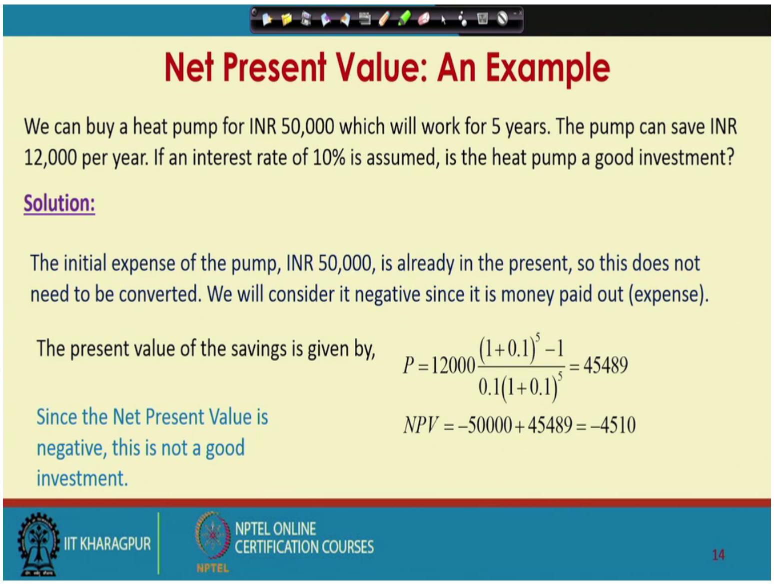
(Refer Slide Time: 31:53)



So, the constraint on cross sectional area is pi capital D square by 4 must be greater or equal to n into small d square and then of course, you have non negativity constraint on 4 decision variables which must be greater or equal to 0. So, this is how you will the optimization problem for economic optimization of shell and tube heat exchanger design we now briefly talk about a concept known as net present value. One approach to evaluate the economics of a project or a decision is to use net present value NPV; here we convert all economic transactions to equivalent values in the present. In general expenses or outflows are considered negative inflows or savings or income are considered positive.

So, there are 2 formulas this formula tells you that if the present value P of one future payment of receipt F at period n with interest rate i is P equal to F n 1 plus i to the power n. Whereas if the present value of a series of uniform payments A where the first payment is made at the end of the first period is given by this expression. So, this equation is useful to find out the present value of say an investment. Let us say I am now investing 1 lakh rupees for 10 years and somebody says that in every year I will give you 12000 rupees.

(Refer Slide Time: 33:55)



So, for 10 years 12000 into 10 I will get 120000 rupees. So, that so whether it is advisable this investment will be profitable or not can be found out from this expression we will take a simple example and it will be clear. We can buy a heat pump for say rupees 50000, which will work for 5 years. The pump can save 12000 rupees per year, if an interest rate of 10 percent is assume is the heat pump a good investment. The initial expense of the pump is 50000 rupees it is already in the present. So, this does not need to be converted it is already expressed in terms of present. We will consider a negative because this is the money we are paying out to buy the heat pump.

So, this is an expense and expense will be considered negative the savings or income will be considered positive. So, now we have to consider we have to consider the present value of the savings. So, we will get 12000 rupees per year we will save 12000 rupees per year for 5 years. So, what is the value of 12000 rupees? If you get 12000 rupees every year and for a period of 5 years what is the present value of that quantity? So, that turns out to be 45000 45489 rupees I make use of the expression given in the previous slide.

So, NPV is now minus 55000 plus 45489 which is minus 4510, so since the net present value is negative this is not a good investment. In fact, if you deposit the money within intercept of 10 percent perhaps you will be better off instead of buying heat pump with this I would like to conclude lecture 10 as well as we conclude with 2 here.