Optimization in Chemical Engineering
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Lecture – 52
Applications of Optimization (Contd.)

Welcome to lecture 52. This is week 11 and in this week we will be talking about Applications of Optimization. In our previous lecture we have talked about the use f min con and f solve, which are solvers available in mat labs optimization tool box. So, we took an example of CSTR s in series and demonstrated the use of f min con and f solve for solution of an optimization problem.

Specifically we had 3 CSTR s in series and a reaction of the type a to products was taking place in each of these reactors. So, you want to find out the optimal values of the volumes of the CSTR so that the concentration of the reactant a in the exit stream of CSTR (Refer Time: 01:21) is minimized. In other words we wanted to convert the maximum amount of a to products. So, today also we will take similar examples and continue our discussion on applications of optimization.

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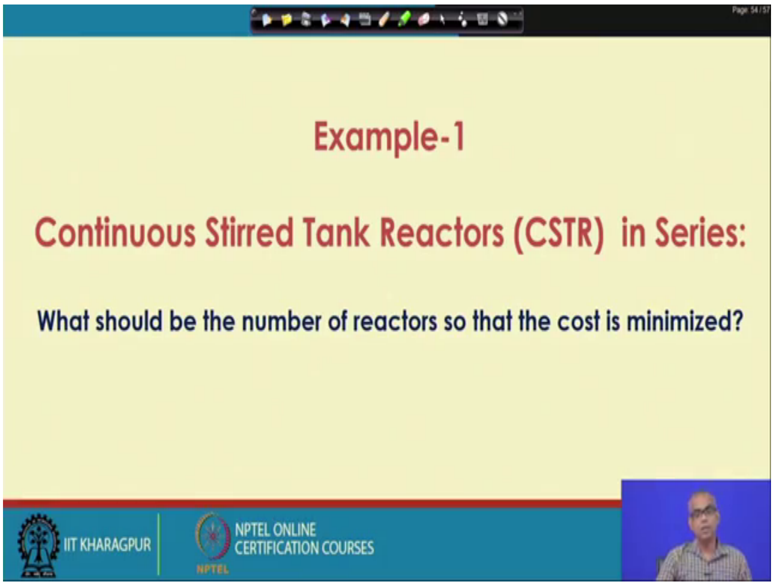

So, as first example, we are again taking the case of continuous stirred tank reactors in series, but this time we are thinking that there are n number of reactors in series; each reactor has the same volume and we want to find out the optimum number of the reactors in the strain so that the total cost is minimized for a specific change in concentration of the inlet reactant stream.

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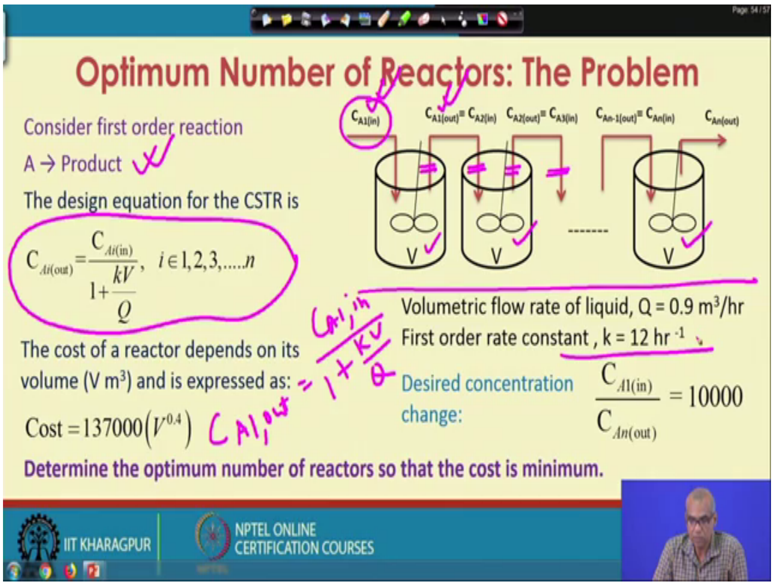

So, let us try to understand the problem first. So, we have n number of CSTR s in series. So, an inlet stream with concentration C A1 in enters CSTR 1. The first order reaction A to products is taking place in each of this CSTR s. So, the outlet concentration of CSTR 1 is the inlet concentration of CSTR 2. The outlet concentration of CSTR 2 is the inlet concentration to CSTR 3 and so on and so forth.

The design equation for the CSTR is given as C Ai out equal to C Ai in divided by 1 plus kV by Q for i equal to 1 2 3 up to n. So, if we want to write let us say for the first reactor CSTR, will write as C A 1 out equal to C A 1 in divided by 1 plus kV by Q similarly you can write for CSTR 2, 3 so on and so forth.

Now, CA 1 out is the outlet concentration of CSTR 1; CA 1 in is the inlet concentration to CSTR 1, k is the first order rate constrained which is given as k equal to 12 hour inverse, V is the volume of each reactor b meter cube and Q is the volumetric flow rate of these streams which is 0.9 meter cube per hour. So, the volumetric flow rate of the stream Q equal to 0.9 meter cube per hour is fixed for all the reactors.

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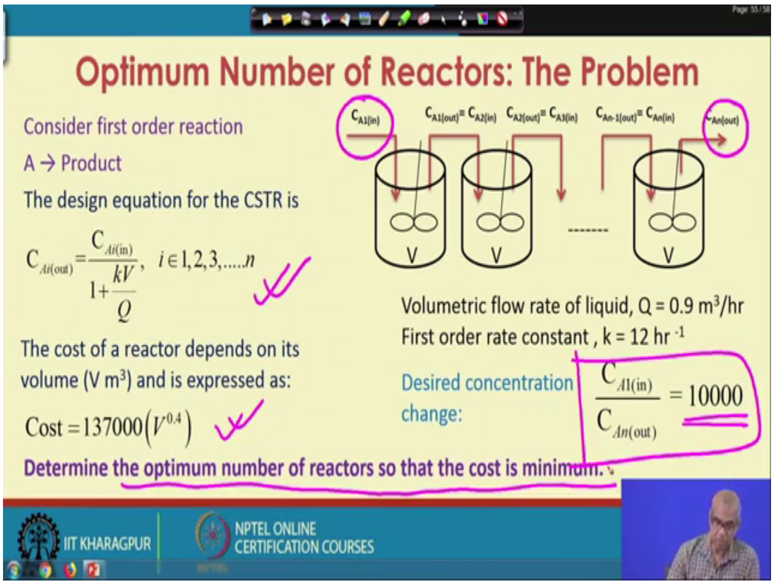

So, that we understand the design equation for the CSTR. The cost of a reactor depends on its volume and is expressed as cost equal to 137000 into V to the power 0.4. The desired concentration changes C A 1 in by C A n out will be 10,000. So, this concentration divided by this concentration will be equal to 10,000.

So, we want that, if we have n number of CSTR s in series. The outlet concentration the concentration of a in the outlet stream will be 1 by 10000 of the inlet concentration of A into the CSTR 1. So, this is my desired concentration change. So, I have to find out the optimum number of reactors in the train so that the cost is minimum. So, find out the optimum number of CSTR s.

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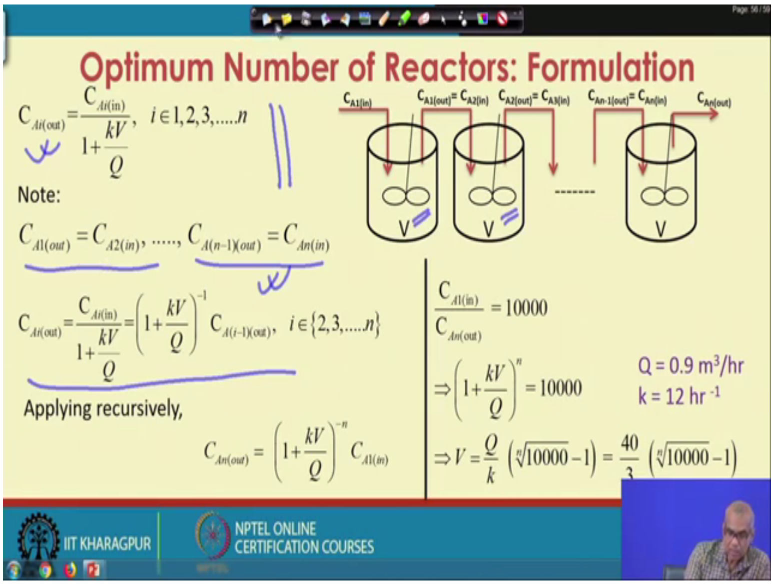

So, this was the design equation C A i out equal to C A i in divided by 1e plus kV by Q; now you understand that the outlet concentration of a CSTR is the inlet concentration to the next CSTR. So, C A 1 out equal to CA 2 in; C A 2 out equal to CA 3 in up to C A n minus 1 out equal to C A in.

So, now combining this and this then we can write that C i out equal to C i in by 1 plus kV by Q and this C A i in.

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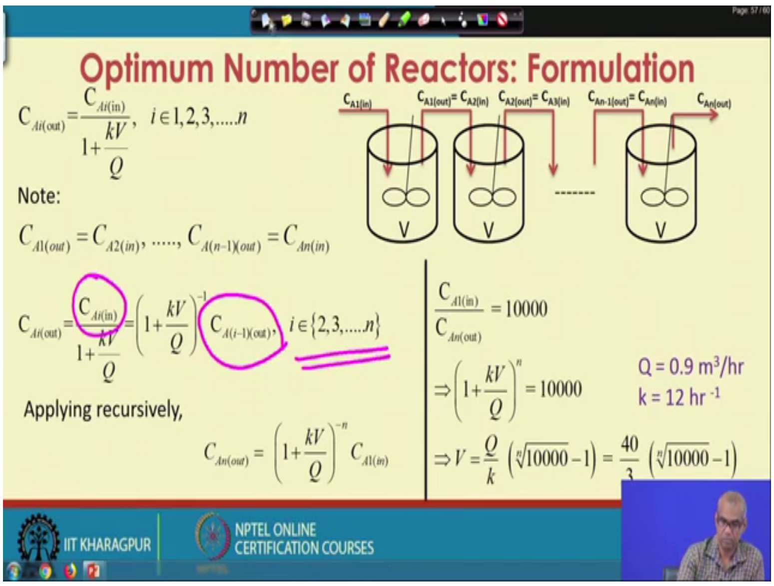

This C A i in is basically C A i minus 1 out. We know that the inlet concentration to a particular reactor number i is basically the outlet concentration of the reactant i minus 1. So, C A i in equal to C A i minus 1 out. Note that this is valid for i equal to 2 3 up to n starting from 2.

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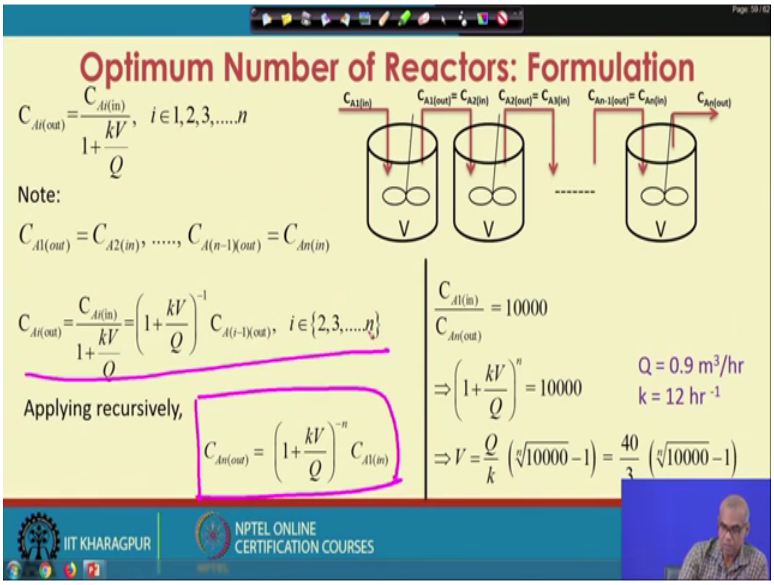

So, now if we apply this recursively we will be able to write CA n out equal to 1 plus kV by Q to the power minus n C A 1 in. What will happen basically is if you use these things recursively, you will be able to write C A 1; note this how this C A n out and C A 1 in are related. This equation needs to be applied recursively.

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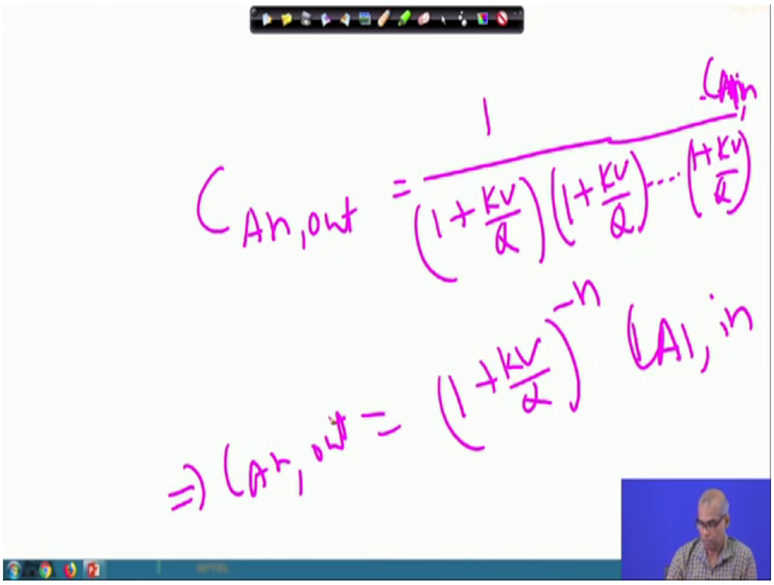

If you do that what will get is C A n out 1 by 1 plus kV by Q 1 plus kV by Q in such term when you have here C A 1 in. So, this leads to 1 plus kV by Q to the power minus n C A 1 in. So, that is what you get this expression.

Now, what is the desired change? C A 1 in by C A n out equal to 10,000. So, from this to you get 1 plus kV by Q whole to the power n equal to 10,000 note that n is the number of CSTR units in series. Q is given as 0.9 meter cube per hour k is given as 12 hour inverse.

So, from this we can get an expression of V. So we get V equal to 40 by 3 square root n 10,000 minus 1. So, I have been able to space V as a function of n; note that this V is the volume of each reactor.

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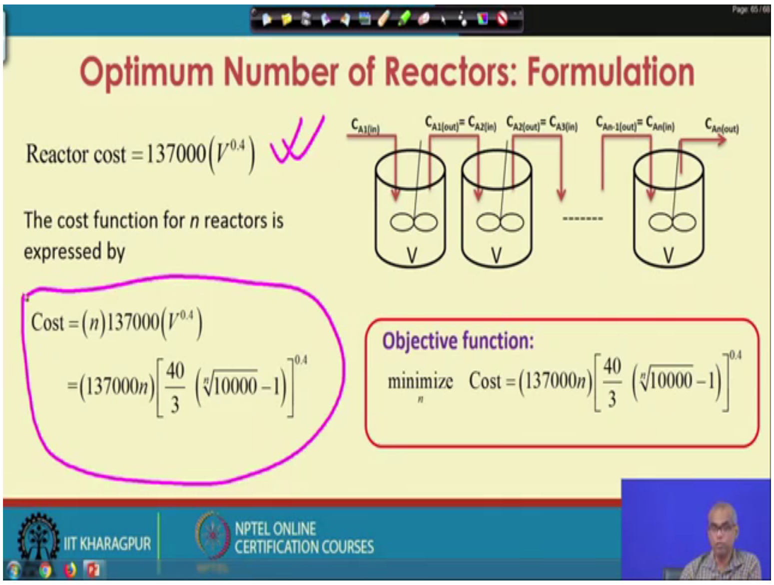

Now, the reactor cost is given as 137000 into V to the power 0.4 this is for each reactor. So, for n reactors you must multiply this by n. So, the cost explanation is cost equal to n into 137000, V to the power 0.4, now we have been able to relate V with n here. So, let us substitute V so, that is what we are doing here. So, why substituting the relationship of V and n were able to express the cost expression as a function of n alone.

So, to find the minimize cost, we now have to find the value of n that minimizes the cost as represented by this expression. So, note we have an unconstrained function of single variable. So, my objective function is minimize the cost function find out n and minimize the cost function.

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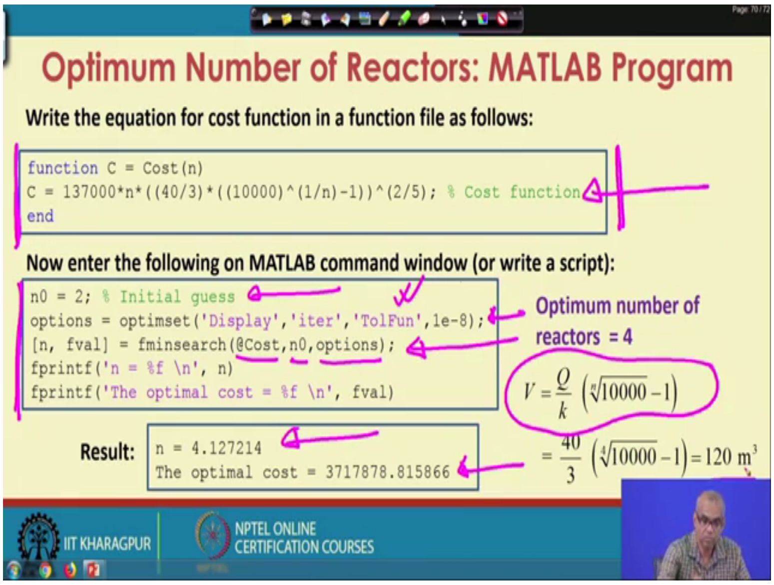

So, we have this unconstrained minimization problem in single variable, we can use f min search of MATLAB optimization toolbox to solve this problem. If you remember f min search uses simplex algorithm to solve the problem. So, first thing, you write the equation for the cost function in a function file as shown here. So, I define a function called cost function c equal to cost of n, and there I am writing the expression for the cost which is the function of n. And n is the decision variable; that means, the number of CSTR units which are connected in series optimum number of CSTR's. Now you write these expressions on mat lab common window or write a script and run the script.

So, give the initial guess let us start with a guess that n equal to 2. So, n 0 equal to 2 you can give the options to display the results of each iterations and to define the tolerance and then you call f min search solver using f min search at cost. So, name of the function where you are defining the cost n 0 is the initial case and options is instruction to the solver to display the results and to set the tolerance at 10 to the power minus 8.

The output will be m which is the optimal number of CSTR units, and f 1 is the function value at this optimal number of CSTR units; that means, the cost associated with the optimal number of CSTR units. See if you run this program you will get n equal to 4.12 as the minimum optimal value of n. And the optimal cost associated with n equal to 4.12 is 3717000 something.

So, although the value is slightly greater than 4.12, we can let us say consider the optimum number reactors that are required is 4. So, if you consider that the volume of each reactor can be computed now, because we know the relationship between the volume and the number of CSTR s in and this gives me the volume of CSTR as each CSTR as 120 meter cube. So, this is how we could solve the unconstrained minimization problem associated with the cost minimization of a CSTR train.

So, this number of CSTR (Refer Time: 19:54) series are known as a reactor trains. So, we found out the optimum number of CSTRs required in the series. So, that the total cost is minimized and we obtain the desired change in the inlet concentrations.

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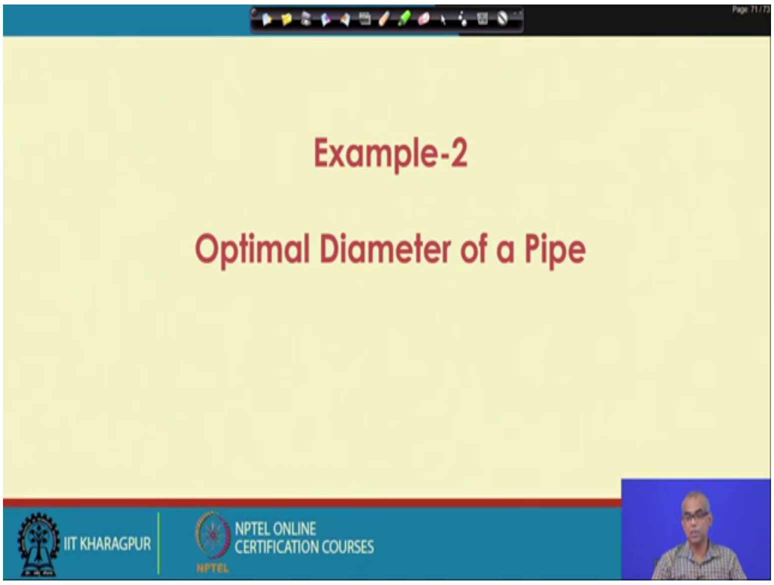

As an second example, let us find out the optimal diameter of a pipe.

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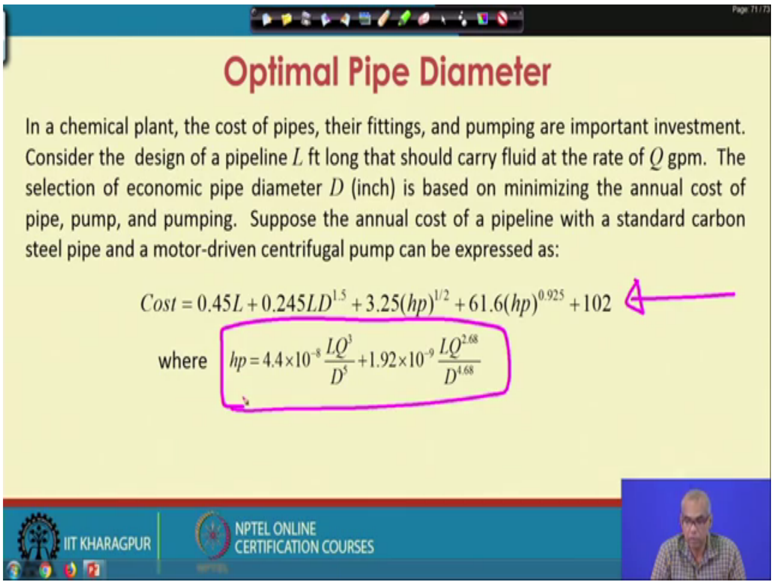

In a chemical plant the cost of pipes their fittings and pumping are important investment. Consider the design of a pipeline L feet long that should carry fluid at the rate of Q gallon per minute. The selection of economic pipe diameter D in inches is based on minimizing the annual cost of pipe pump and pumping. Suppose the annual cost of a pipe line with the standard carbon steel pipe and a motor driven centrifugal pump can be expressed as: this expression.

So, the annual cost is expressed as a function of the pipeline length L, the pipe diameter D and hp associated with the motor, where hp is given by another expression, which is a function of L the pipeline length, D the pipe diameter and the flow rate of the liquid Q.

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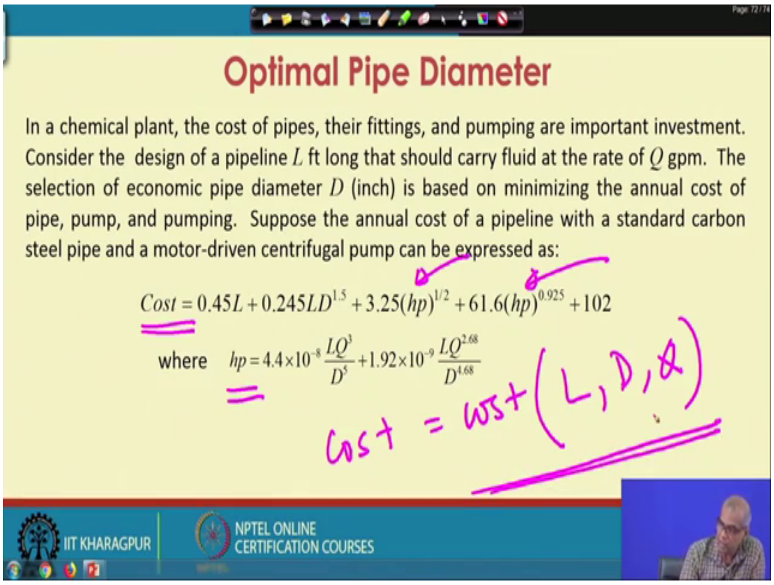

So, basically the cost can becomes a function of L D and Q because hp is a function of L D and Q. So, if this hp is substituted the cost becomes a function of L D and Q.

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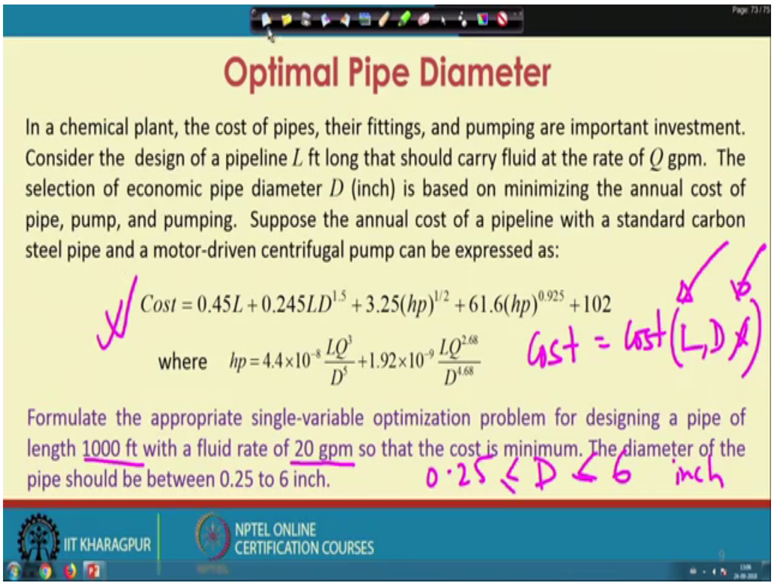

So, let us formulate an appropriate single variable optimization problem for designing a pipe of length 1000 feet with a fluid rate of 20 gallon per minute so, that the cost is minimum.

The diameter of the pipes should be between 0.25 to 6 inch. So, we found that the cost is basically a function of L, D and Q. Now we are specifying the pipe length L at 1000 feet and the Q the flow rate we are specifying at 20 gallon per minute. So, basically the cost becomes now function of 5 diameter alone. So want to formulate an appropriate single variable optimization problem for designing a pipe length of 1000 feet with a fluid rate of 20 gallon per minute so, that the cost is minimum. And you also have a lower bound and upper bound on the pipe diameter. So, the pipe diameter should be between 0.25 to 6 inch and the cost is given by this expression.

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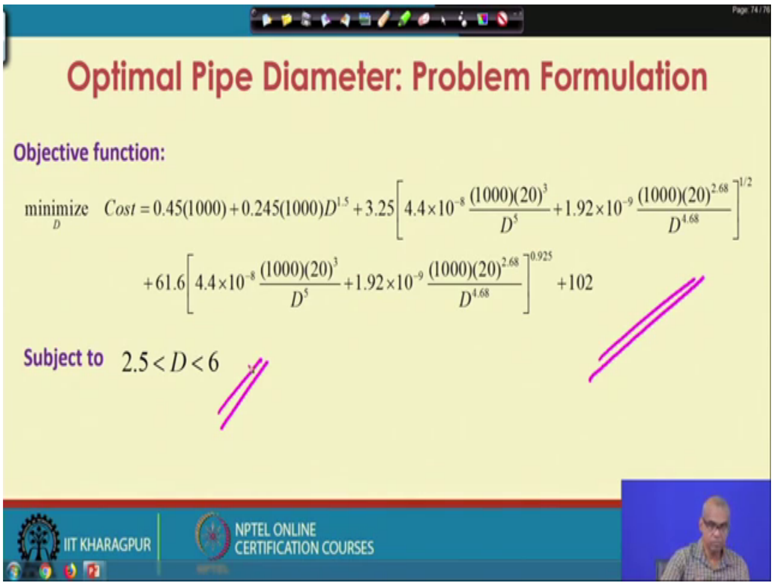

So, there is now straight forward to identify the objective function, the objective function is nothing, but the cost. So, after you have replaced the expression of hp into the expression of cost and substituted L equal to 1000 and Q equal to 20 you will obtain this expression as an expression for cost. And we have bounds on D because D has to lie between 2.5 and 6.

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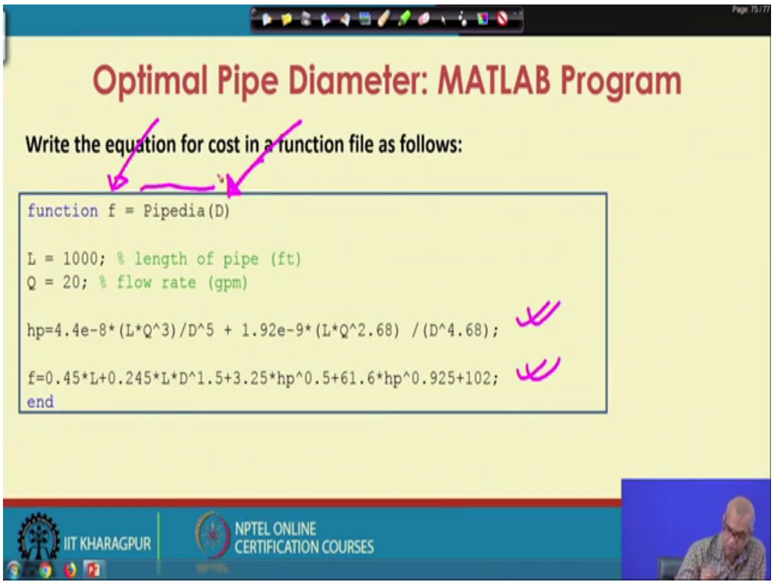

So, to solve let us first write the equation for the cost in a function 5. So, let us write down the function 5. So, I define a function call pipe dia. So, function f equal to pipe dia argument is D; D is the pipe diameter. So, this is the expression for hp and this is the expression for the cost. So, this is equal to f. So, output of this function is the cost for given pipe diameter D.

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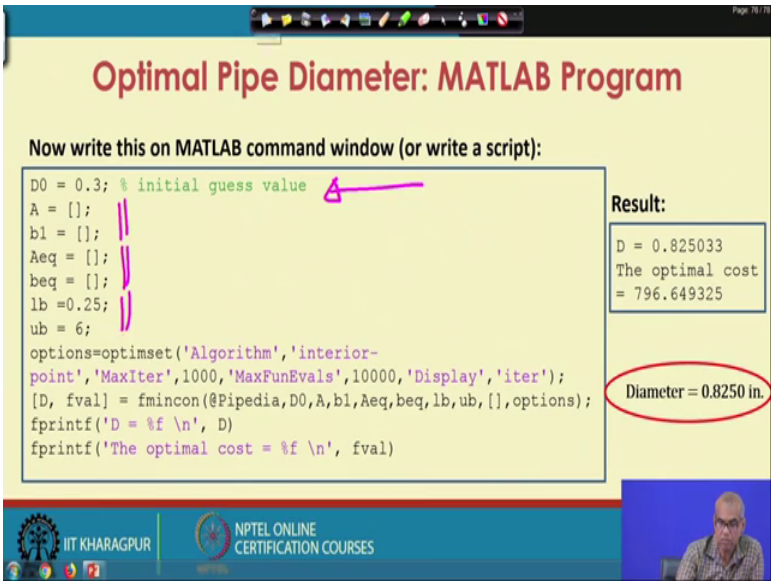

So now, you can use f min con to solve this optimization problem define the. So, you initial guess, we do not have any linear inequality or linear equality constraints, these are the bounds on the decision variable D has to lie between 0.25 and 6 inch.

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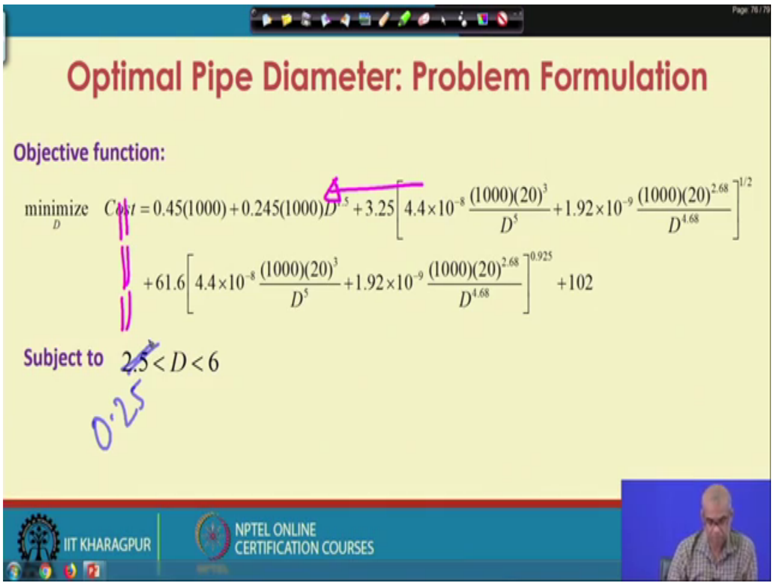

So, this is 0.25 then, I erase this that there is an upper bound and lower bound on the decision variable.

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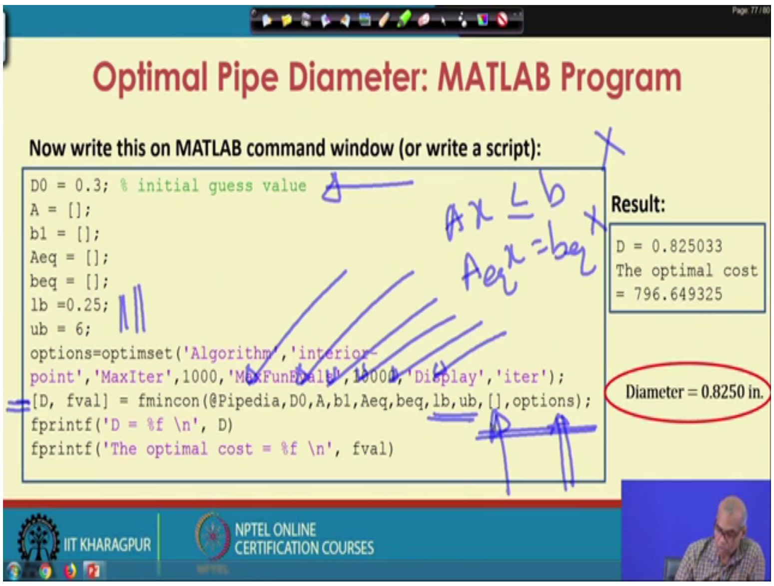

So, you do not have any linear inequality or linear equality constraint, we have an upper bound and lower bound on the decision variable x. So, now, you call the f min con solver following the appropriate syntax. So, first is the name of the function file, which will written the objective function value next stage the initial guess for the solution

So, initial guess for the pipe diameter next A and b 1 corresponds to A x less or equal to b which I do not have. Then next two are for A equality x equal to b equality which again I do not have and then we have lower bound and upper bound and we have defined those as l b equal to 0.25 and b equal to 6.

I do not have non-linear constraints so, supplied null and then options. We have supplied options to define maximum function evaluations 10,000 and to display the results at each iteration. So, the output it gives is the optimal pipe diameter and the function value at this optimal diameter; that means, cost at this optimal diameter. So, the result is D equal to 0.825033, and the optimal cost is 796.64 in appropriate unit. So, the optimal diameter is obtained as 0.8250.

So, this was an unconstrained single variable optimization problem. So, in this lecture we talked about 2 single variable un constrained optimization problem. The first one is solved using f min search that was a problem where you found out the optimal number of CSTR s in the reactor train. And next again we solve a single variable un constrained problem, but this time you solved using f min con.

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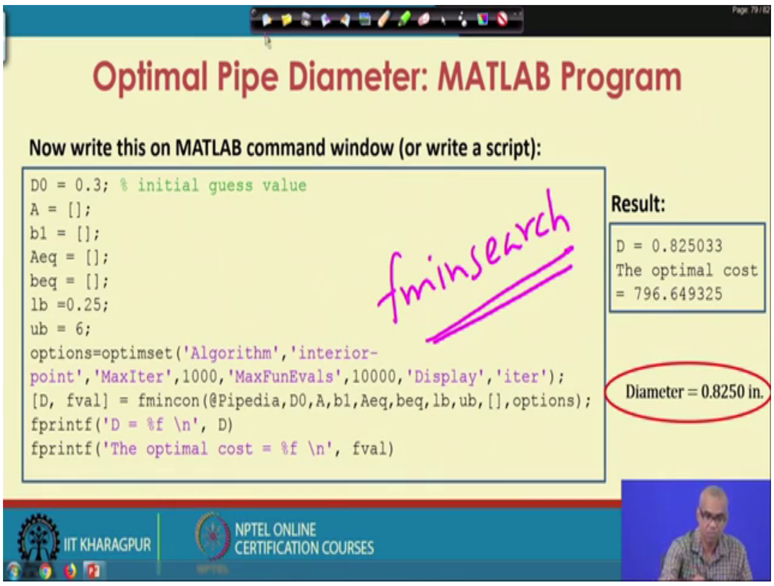

So, you can also solve this problem using f min search, and I will suggest that you solve this problem using f min search as well and compare the results.

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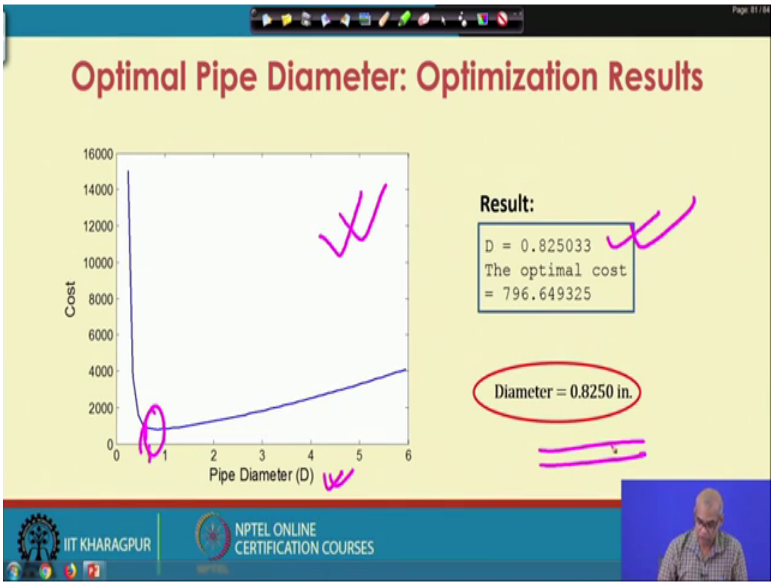

So, this is if you draw the cost buses the pipe diameter.

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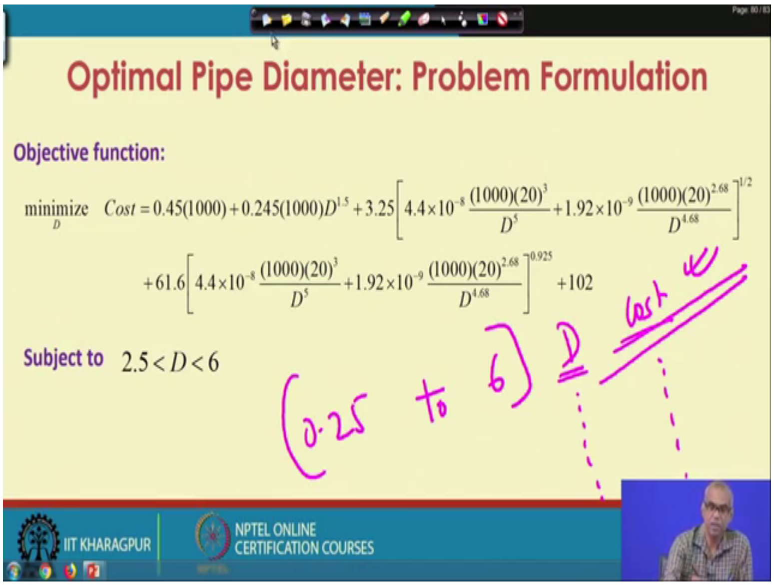

See you basically have an expression for cost versus diameter. So, what you can do is between 0.25 to 6 inch, you can generate the D values and can obtain the corresponding the cost values using this expression.

And then if you plot, you will get this plot. So, this plot is nothing, but the direct use of the cost function expression for various values of the pipe diameter D. So, this is since this is a single variable optimization problem, you can obtain the optimal value of D simply by plotting. So, we can see that here also the value is above 0.82 so, the minimum lies here.

So, we will have confidence in our results and we conclude the optimal pipe diameter is 0.8250 inch. So, with this we will come we conclude our lecture 52 here.