Plant Design and Economics
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Lecture No -35
General Procedure for Reactor Design and Cost Estimation

Welcome to lecture 35 of plant design and economics, in this last lecture of module 7 we will have a discussion on general procedure for reactor design and cost estimation of reactors.

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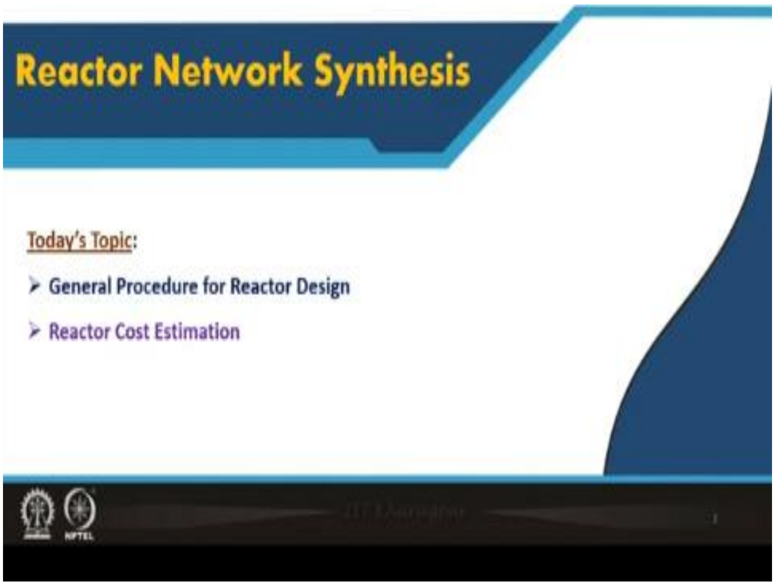

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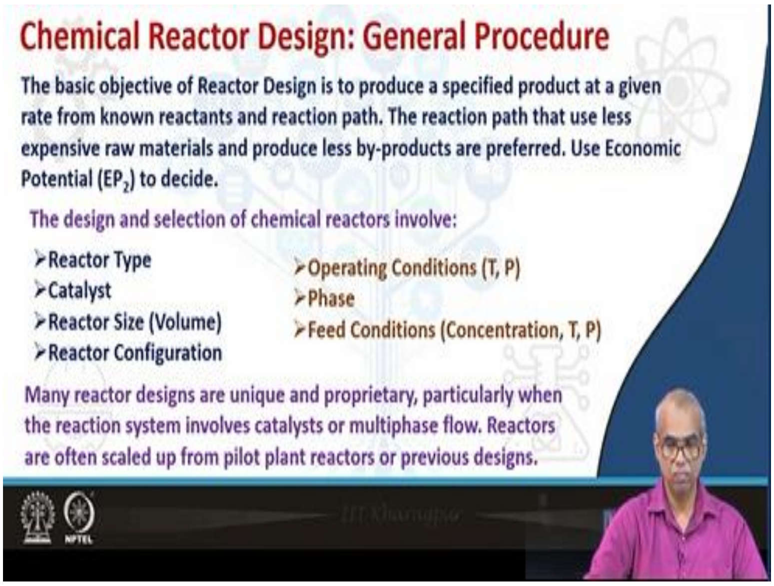

The basic objective of reactor design is to produce a specified product at a given rate from known reactance and reaction path. The reaction paths that use less expensive raw materials and produce less by products are preferred. So we can use economic potential to decide this. These are economic potential we have discussed when we talked about conceptual process synthesis.

The design and selection of chemical reactors involved reactor type, catalyst, reactor size or volume, reactor configurations, operating conditions, such as temperature, pressure, phase, feed condition that is concentration, temperature, pressure of feed. Many reactor designs are unique and proprietary in nature, particularly when the reactions came involves catalysts or multiphase flow.

Reactors are not always designed starting from the first principles; reactors are often designed by scaling it up from pilot plant reactors or previous designs.

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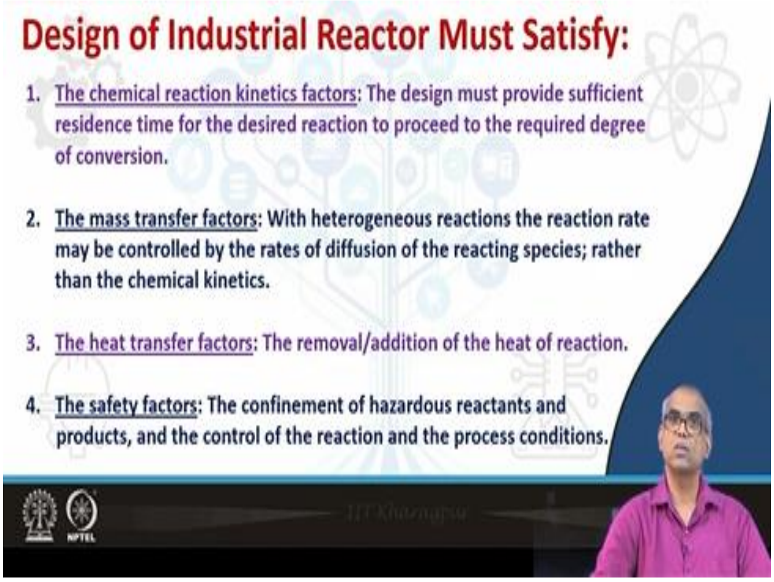

Design of industrial reactor must satisfy the following points: the chemical reaction kinetics factors: The design must provide sufficient residence time for the desired reaction to proceed to the required degree of conversion. The mass transfer factors: with heterogeneous reactions the reaction rate may be controlled by the rates of diffusion of the reacting species; rather than the chemical kinetics.

The heat transfer factors: The design must satisfy the removal or addition of the heat of reaction. The safety factors: The design of reactors must satisfy the confinement of hazardous reactants and products and the controller of the reaction and the process conditions for safe operations.

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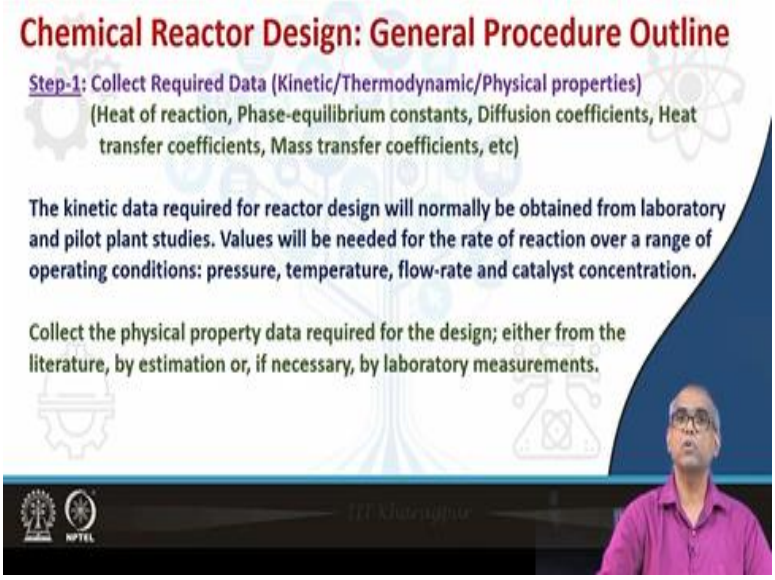

Now, let us outline the general procedure for chemical reactor design. In the step 1 collect required data, kinetic data, thermodynamic data, physical properties, etcetera the data that are important are heat of reaction, phase-equilibrium constants, diffusion coefficients, heat transfer coefficients, mass transfer coefficients etcetera. The kinetic data required for reactor design will normally be obtained from laboratory and pilot plant studies.

It is not very likely that you will obtain data for commercially attractive processes in open literature because such data are generally protected for business interest, so the kinetic data required for reactor design will normally we obtained from laboratory and pilot plant studies. Values will be needed for the rate of reaction over a range of operating conditions such as pressure, temperature, flow-rate and catalyst concentration.

Collect the physical property data required for the design this can be collected from literature or it can be estimated by using various models and correlations or you can also perform laboratory experiments to obtain such data.

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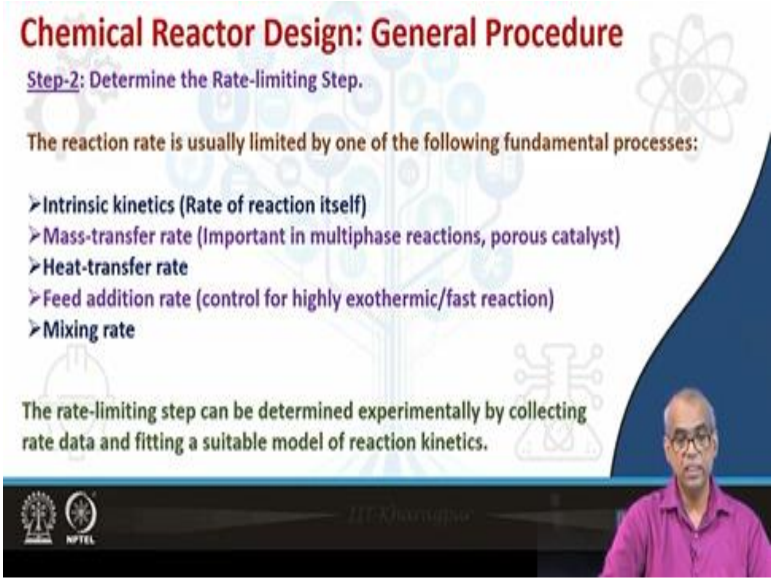

In the step 2, determine the rate limiting step: the reaction rate is usually limited by one of the following fundamental processes, the intrinsic kinetics that is rate of the reaction itself. Mass transfer rate, mass transfer rate is limiting particularly in multiphase reactions or in presence of porous catalyst where the diffusion of the species is involved. Heat transfer rate may be limiting, feed addition rate may be limiting.

By manipulating the feed addition rate, we can effectively control highly exothermic reactions or reactions that occur very fast, mixing rate can also be rate limiting. So, how do you find out which one is the rate limiting step? This can be determined experimentally by collecting rate data and then fitting a suitable model for reaction kinetics. So assume a rate limiting step solve the model try to feed the rate data and this way you can experimentally determine what will be the rate limiting step.

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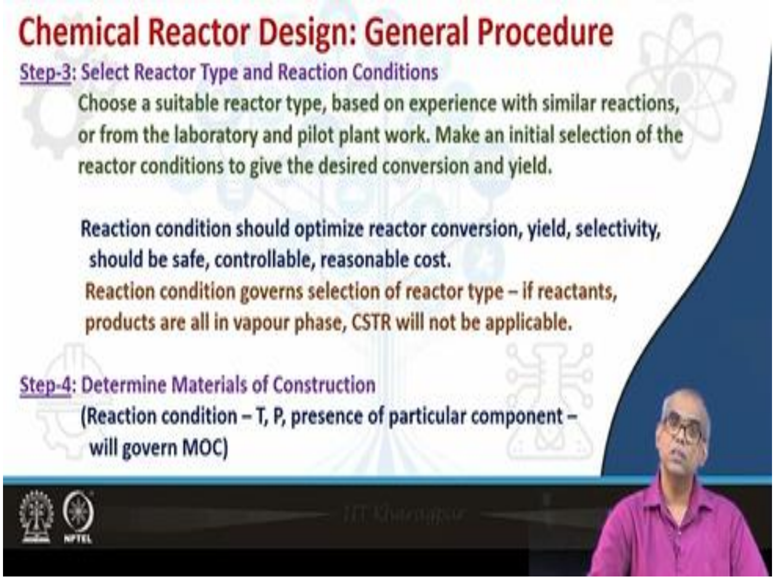

Once you have determined rate limiting step you select reactor type and reaction conditions choose a suitable reactor type based on experience with similar reactions or from the laboratory and pilot plant work. Make an initial selection of the reactor conditions to give the desired conversion and yield. Reaction conditions should optimize reactor conversion, yield, selectivity, reacting conventions should be safe, it should be controllable.

And, this conditions must be achieved at a reasonable cost, reaction conditions governs selection of reactor type. For example, the reactance products are all in vapour phase the CSTR will not be chosen. Then we can determine the materials of constructions: The factors that govern the choice of material of construction will be reaction conditions such as temperature, pressure, presence of particular component will govern material of constructions it may be required that you make use of special alloy.

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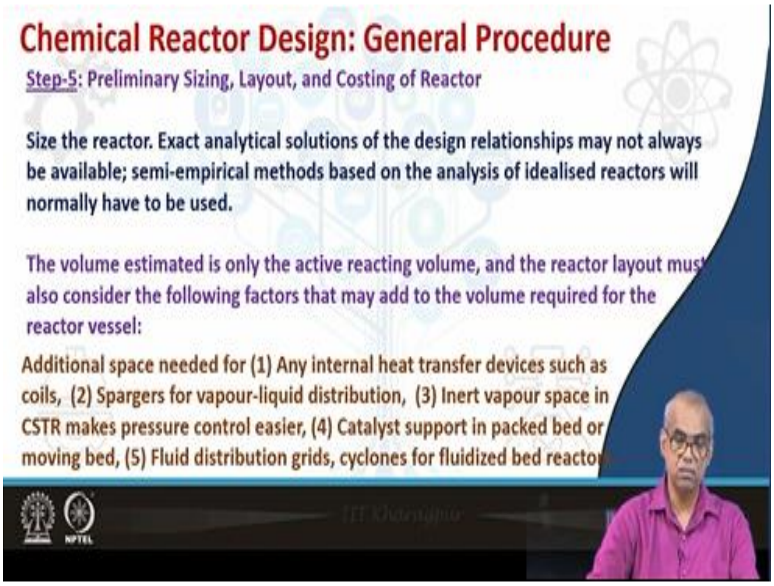

In step 5, you can perform preliminary sizing, layout and costing of reactors. While sizing the reactor, exact analytical solutions of the design relationship may not always be available. So, semi-empirical method based on the analysis of idealized reactors will have to be used often. The volume estimated is only the active reacting volume and the reactor layout must also consider various factors that may add to the volume required for the reactor vessel.

So, what are those factors? Additional space needed for any internal heat transfer devices such as cooling coils, heating coils within the reactor, spargers for vapour-liquid distribution, inert vapour space; inert vapour space in CSTR makes pressure control easier, catalyst support in packed bed or moving bed, fluid distribution grids, cyclones for fluidized bed reactor. So, we must add extra volume for these factors.

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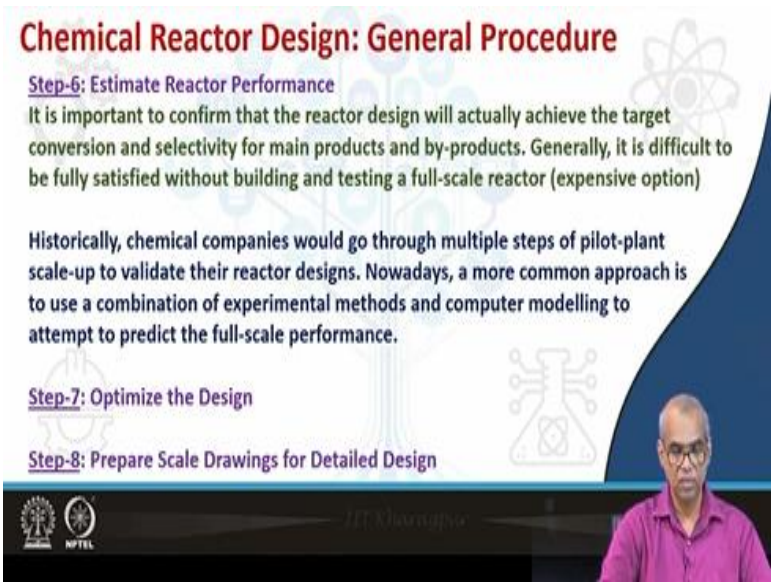

Next, we estimate reactor performance: it is important to confirm that the reactant design will actually achieve the target conversion and selectivity for main products and by products. Generally, it is difficult to be fully satisfied without building and testing a full scale reactor, which is economically expensive option. Historically, chemical companies would go through multiple steps of pilot plane scale up to validate their reactor design.

However, currently we can perform simulation studies and follow a combine approach of experiments as well as mathematical modelling and computer simulation to attempt to predict the full scale performance, this saves both time and money. The steps 7, we optimize the design at this stage it may be necessary that we go back to some of the previous steps and redo the calculations.

In this final in the step 8, we prepare scale drawings for detailed design. So these are the outlines of general procedure for chemical reactor design.

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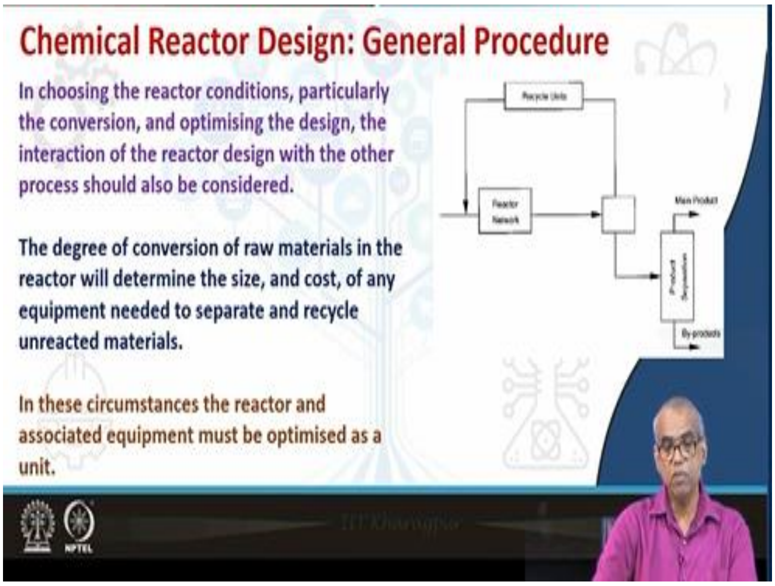

Now, only choose reactor conditions particularly the conversion and optimize the design we should also keep in mind the interactions of the reactor or reactor networks with the other process units in the process flow sheet, particularly the separation units. The degree of conversion of raw materials in the reactor will determine the size and cost of any equipment needed to separate and recycle un-reacted materials.

So, the conditions in the reactor will heavily influence the recycle as well as the separation units. So a better way to optimize the reactant network or reactors will be that we consider the optimization of reactor separation system together, so we consider reactor separation system as one unit and then optimize the process.

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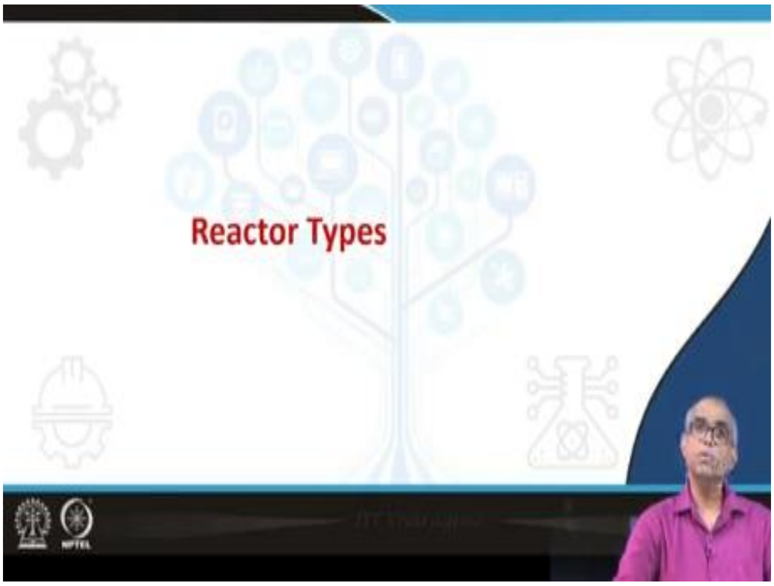

Now, we will briefly talk about few reactor types.

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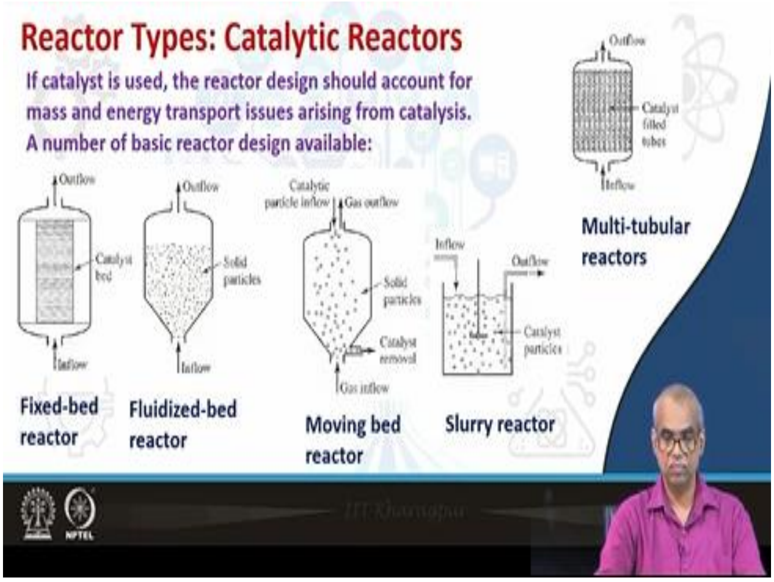

Catalytic reactors; if catalyst is used the reactor design should account for mass and energy transport issues that arise due to the presence of catalyst. A number of basic reactor designs are available such as fixed bed reactor, fluidized bed reactor, moving bed reactor, slurry reactors and multi-tubular reactors. So these are commonly used catalytic reactors. In all these reactors, we use solid catalysts.

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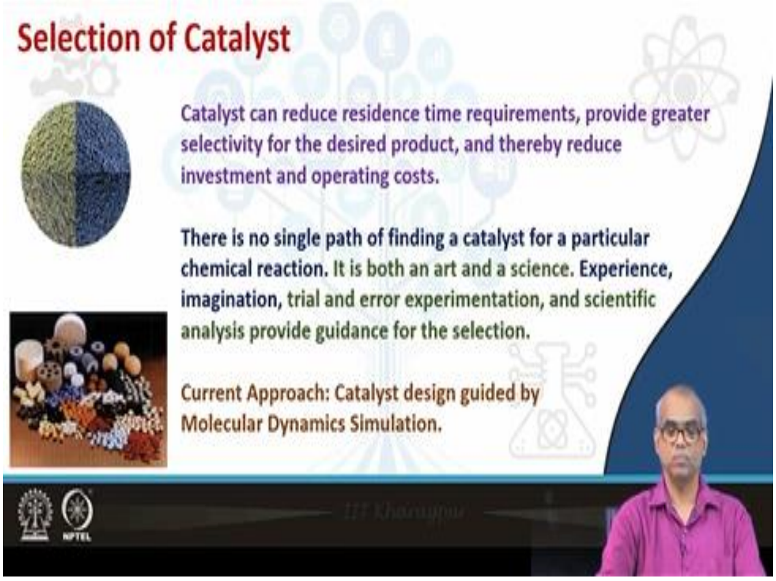

Catalyst can reduce residence time requirements, provide greater selectivity for the desired product and thereby reduce investment and operating cost. How do you select the catalyst? What will be the most appropriate catalyst for my process? Unfortunately, there is no single path of finding a catalyst for a particular chemical reaction. It is both an art and science to find the appropriate catalyst for any given process.

Experience, imagination or creativity, trial and error experimentation and scientific analysis of the experimental results will provide guidance for the selection. Currently, catalyst designs are guided by molecular dynamic simulations. So molecular dynamic simulations is helping a big way for design of new catalyst, again this helps in saving time as well as money.

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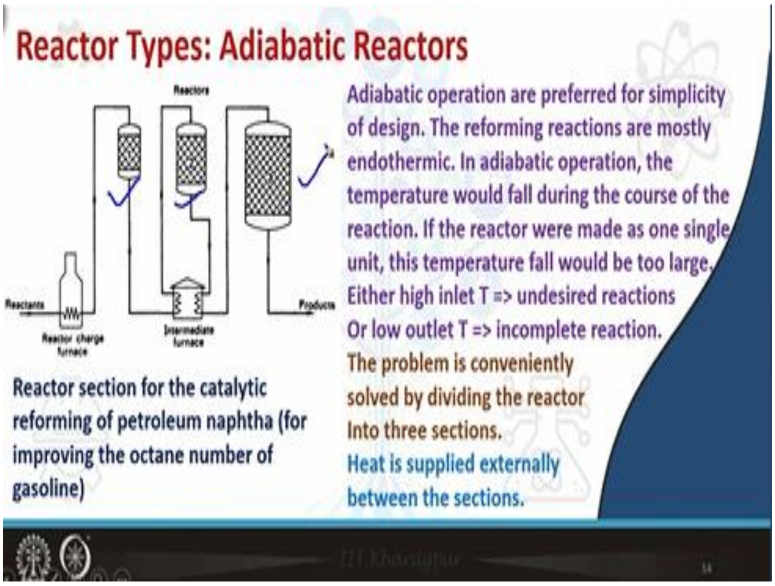

What you see in figure is the reactor section for the catalytic reforming or petroleum naphtha, the reforming of petroleum naphtha is done for improving the octane number of the gasoline. Adiabatic operations are preferred for simplicity of design. The reforming reactions are mostly endothermic, so during adiabatic operation the temperature would fall during the course of the reaction.

If the reactor is made as one single unit then this temperature fall may be too large, so to have this we can increase the inlet temperature otherwise we must have the low outlet temperature. So, if you use high inlet temperature this can lead to undesired reactions and undesired by-products, whereas low temperature at the outlet will lead to incomplete reactions, note in the figure the reactors have been divided in three sections, 1, 2 and 3.

And, heat is supplied externally between the sections using intermediate furnace, so such considerations should be there during design process.

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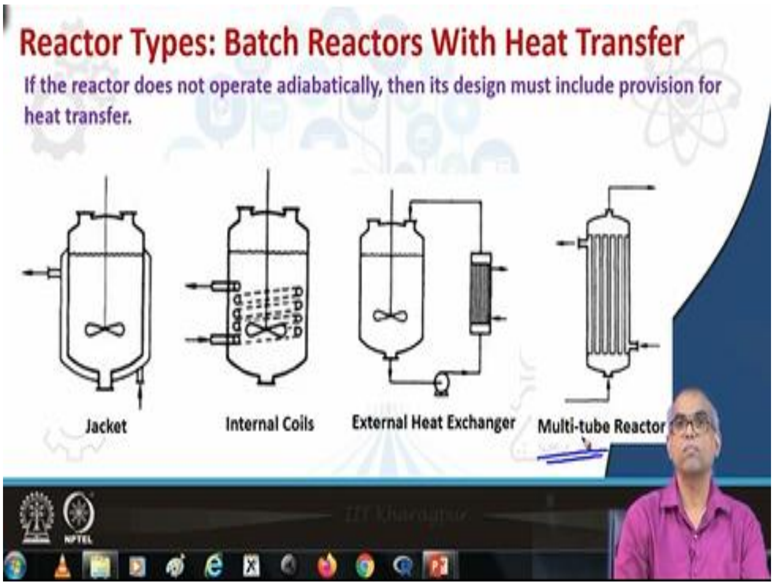

If the reactor does not operate adiabatically then it is design must include provision for heat transfer. Note, the provision for heat transfer in the figures we can use a jacket; cooling jacket or heating jacket around the reactor, we can use internal coils, we can use external heat exchanger or we can also use multi tube reactor.

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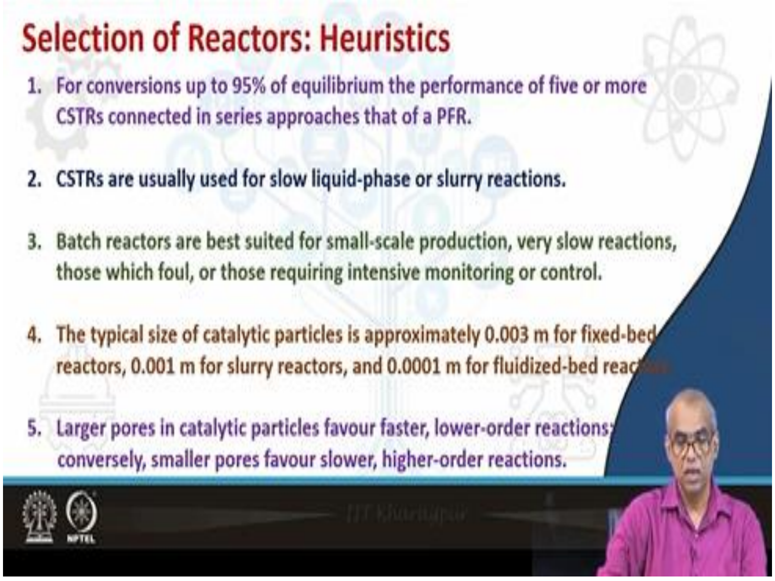

Here are some selections for reactor; here are some heuristics for selection of reactors. For conversion up to 95% of equilibrium the performance of 5 or more CSTR's connected in series approaches that of a PFR. CSTR's are easily used for slow liquid phase or slurry reactions. Batch reactors are best suited for small scale productions, very slow reactions, those with foul, or those requiring intensive monitoring or control.

The typical size of catalytic particles is approximately 0.003 meter for fixed-bed reactors, 0.001 meter for slurry reactors and 0.0001 meter for fluidized bed reactors. Large pores in catalytic particles, favour faster, lower-order reactions conversely, smaller pores favour slower, higher-order reactions. So these are some heuristics for selection of reactors.

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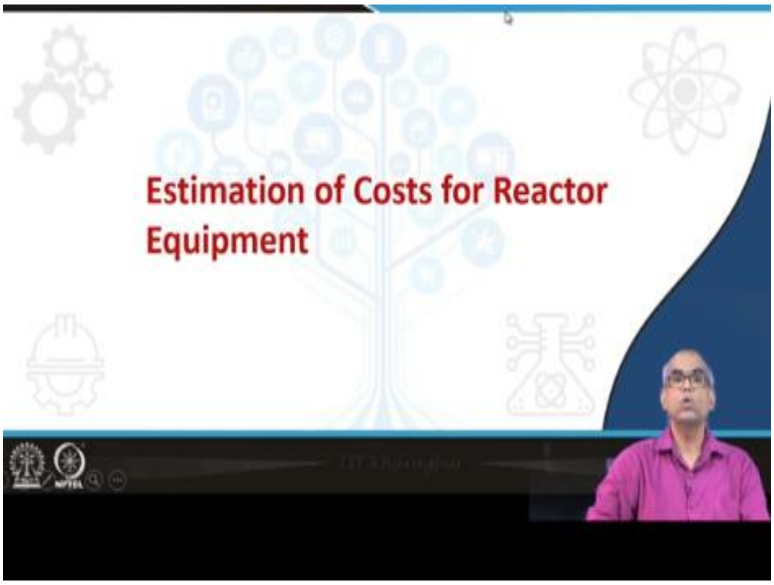

Now we will briefly talk about estimation of cost for reactor equipment.

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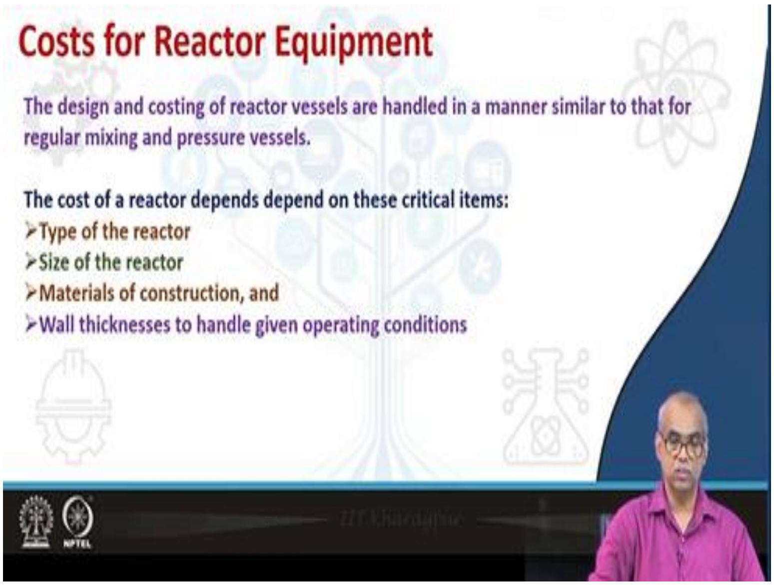

The design and costing or reactor vessels are handled in a manner similar to that for regular mixing and pressure vessels. The cost of a reactor depends on various items such as type of reactor, size of the reactor, materials of construction, as well as wall thickness to handle give operating conditions. Note that, we must choose appropriate materials of construction and wall thickness to handle given operating conditions.

So, the cost of the reactor will depend on all such critical items type and size of the reactor, as well as materials of construction and wall thickness.

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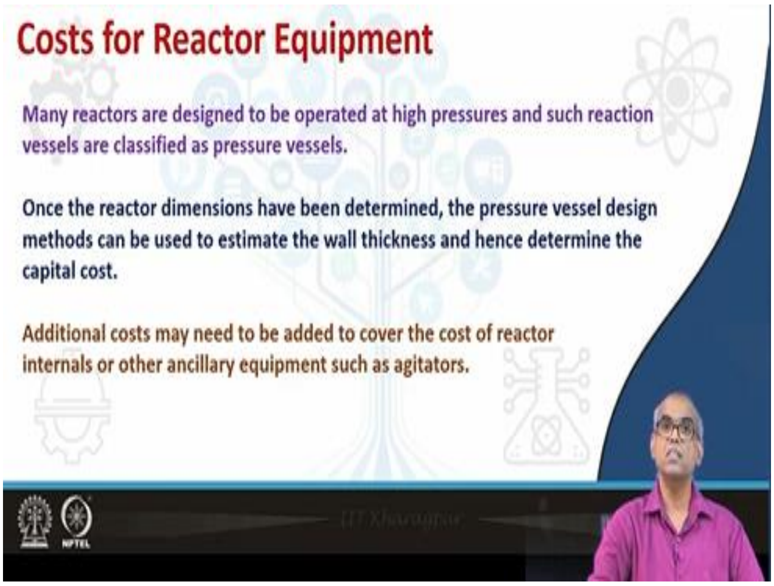

Many reactors are designed to be operated at high pressures and such reaction vessels are classified as a pressure vessels or pressure vessel reactor. Once the reactor dimensions have been determined, the pressure vessel design method can be used to estimate the wall thickness and hence determine the capital cost. Additional cost may be needed because we will require additional cost for the reactor internal as well as for ancillary equipment such as agitators.

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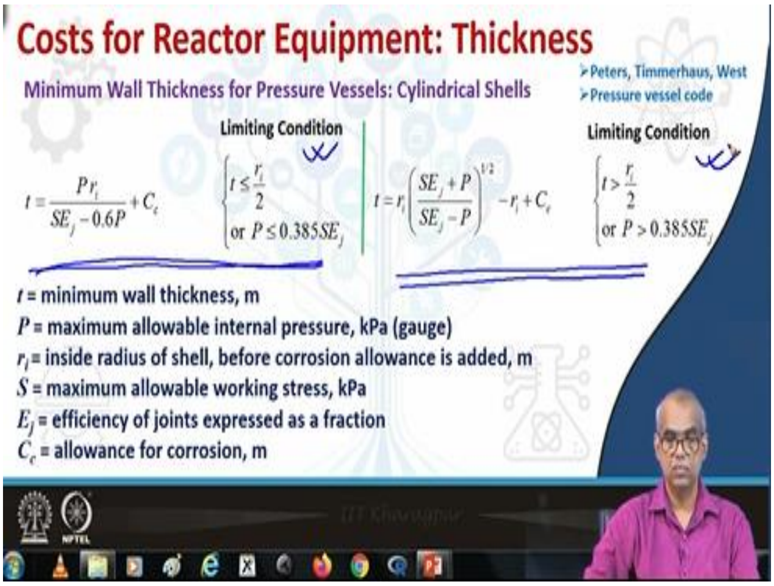

Now you can look at separation vessel codes say semi-pressure visual codes to find out the minimum wall thickness for pressure vessels for various types of cells. For cylindrical cells, the thickness or the minimum wall thickness can be computed using these equations, note these equations are applicable for these given limiting conditions. So you can also look at design books particularly mechanical design, the books for mechanical design to obtain such expressions for minimum wall thickness.

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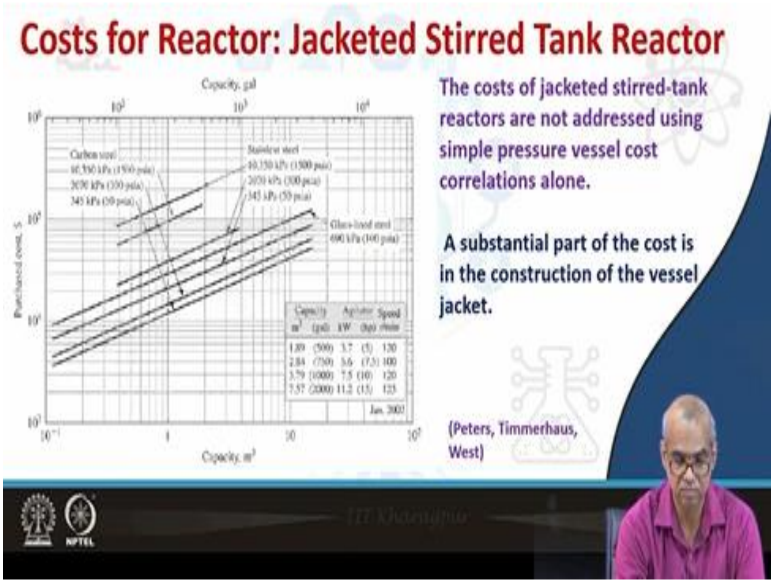

The cost of jacketed stirred tank reactors are not addressed using simple pressure vessel cost correlation alone. The reason is that a substantial part of the cost is in the construction of the vessel jacket. In the figure you see, how the purchase cost and the capacity of the reactors made from various materials of construction, such as carbon steels, stainless steel, gasoline steel are related.

So, such graphical correlations can be used to find out the purchase cost given particular capacity and operating conditions and materials constructions, note that both for carbon steel and stainless steel the data are given for various pressures; 50 psi, 300 psi and 1500 psi. So, such graphical correlations can be used.

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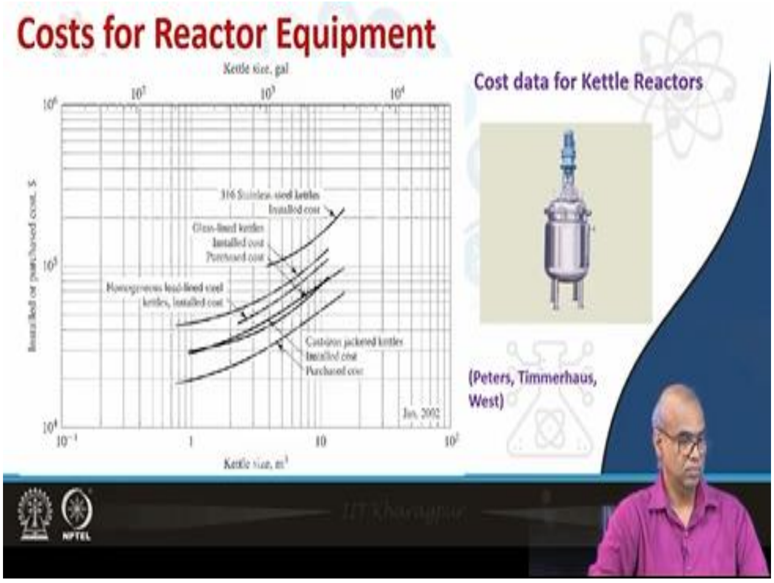

Similar correlations are also available for cost data for kettle reactors.

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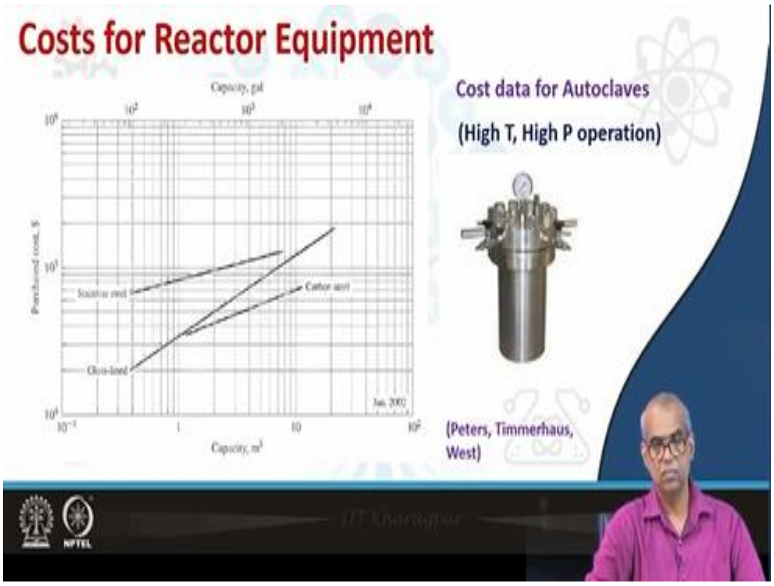

And, also available for autoclaves which are used for high pressure, high temperature applications.

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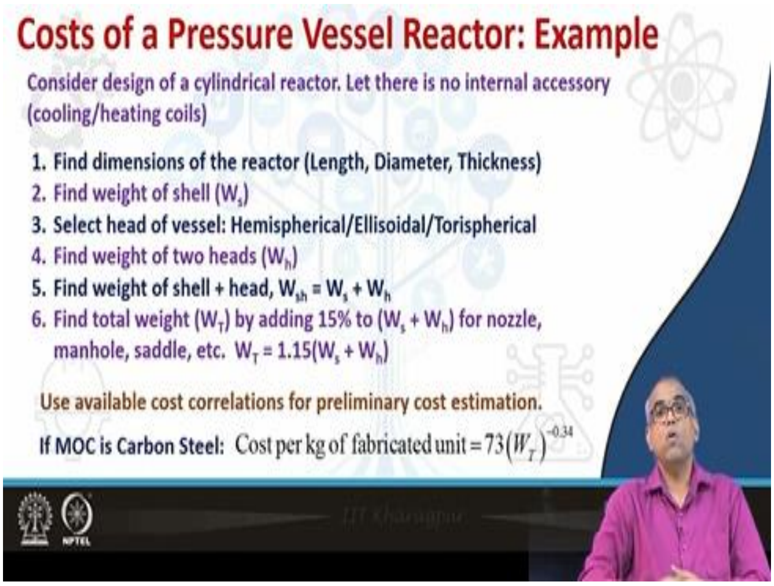

Now, let us look at a very simple example showing the steps to obtain the cost of a pressure vessel reactor. What is we seen the outline of the steps without performing detail calculations, so you are considering the design of a cylindrical reactor and let their, we know internal accessories such as cooling or heating coils. So, how do I obtain the cost of the reactor? So first obtain the dimensions, so size of the reactor, so we get the length and diameter of the reactor then you make use of the code for obtaining the thickness.

We are considering the pressure vessel reactor, so we can look at the pressure vessel code for the cylindrical shell we have given the expression or equation or formula for determination of thickness. So using the procedure for sizing of the reactor and the following the codes for determining the thickness of the pressure vessel reactor, let us consider we have obtained the length, diameter and thickness of the cylindrical shell.

So, now I can find out the weight of the shell, of course at this stage we must know what should be my material of construction and from the density of that we can find out the weight of the shell. Now where I am using a cylindrical shell there will be heads of the shell, so select head of the vessel hemispherical or ellipsoidal or torispherical, let us say we choose hemispherical heads, so we choose hemispherical heads.

So, again consider the design codes for pressure vessels and find out the volume of the two heads and then weight of the two heads, so the find out the weight of the shell plus head. Now, let us add 15% weight of this shell weight plus head weight to take care of nozzle, manholes, saddle etcetera. So, I now obtain the total weight which includes weight of shell, weight of head as well as 15% additional for nozzle, manual, saddle etcetera.

Now, once I have the total weight for the given material of construction I can make use of cost correlations that are available to find out what will be my preliminary cost. So, preliminary cost estimation is possible by obtaining the weight of the reactor material. For example, if material of construction is carbon steel the cost per kg of fabricated unit will be 73 into total weight to the power -0.34.

These expressions are given this particular expression is obtained from the books of Peterson Timmerhaus, so similar cost correlations are available which can be used for preliminary cost estimation purpose. With this we stop our discussion on module 7 here.