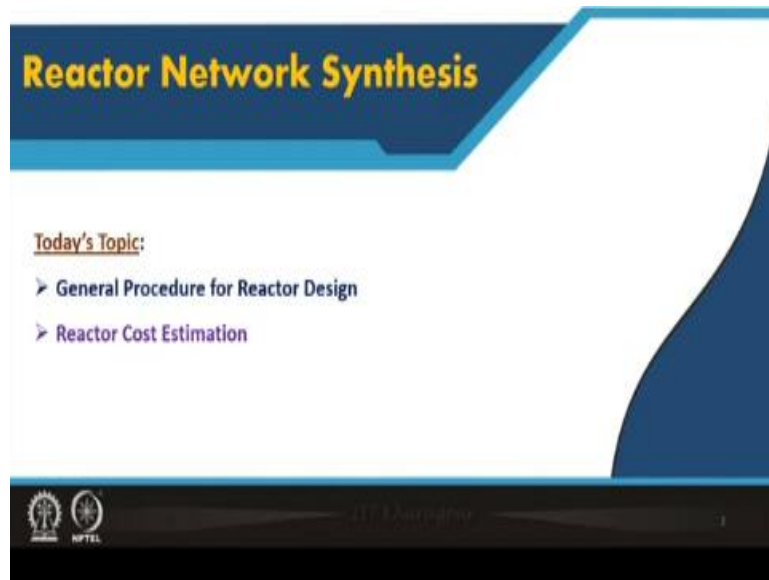


**Plant Design and Economics**  
**Prof. Debasis Sarkar**  
**Department of Chemical Engineering**  
**Indian Institute of Technology, Kharagpur**

**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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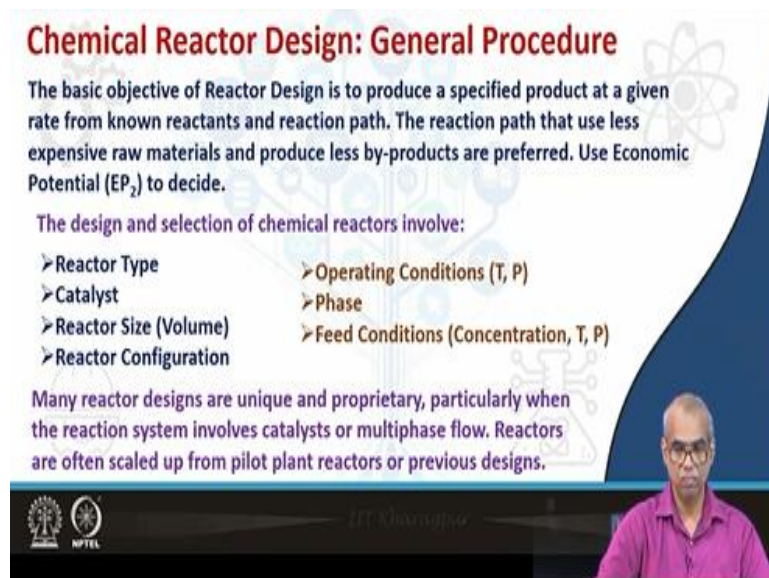
**Reactor Network Synthesis**

Today's Topic:

- General Procedure for Reactor Design
- Reactor Cost Estimation

Logos of IIT Kharagpur and NPTEL are visible at the bottom left.

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**Chemical Reactor Design: General Procedure**

The basic objective of Reactor Design is to produce a specified product at a given rate from known reactants and reaction path. The reaction path that use less expensive raw materials and produce less by-products are preferred. Use Economic Potential ( $EP_2$ ) to decide.

The design and selection of chemical reactors involve:

- Reactor Type
- Catalyst
- Reactor Size (Volume)
- Reactor Configuration
- Operating Conditions (T, P)
- Phase
- Feed Conditions (Concentration, T, P)

Many reactor designs are unique and proprietary, particularly when the reaction system involves catalysts or multiphase flow. Reactors are often scaled up from pilot plant reactors or previous designs.

Logos of IIT Kharagpur and NPTEL are visible at the bottom left. A video inset of Prof. Debasis Sarkar is visible at the bottom right.

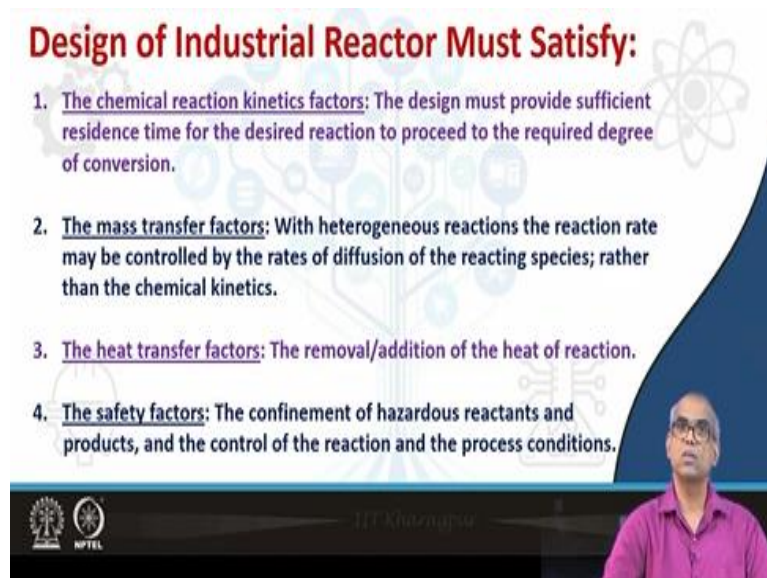
The basic objective of reactor design is to produce a specified product at a given rate from known reactance and reaction path. The reaction paths that use less expensive raw materials

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:**

1. **The chemical reaction kinetics factors:** The design must provide sufficient residence time for the desired reaction to proceed to the required degree of conversion.
2. **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.
3. **The heat transfer factors:** The removal/addition of the heat of reaction.
4. **The safety factors:** The confinement of hazardous reactants and products, and the control of the reaction and the process conditions.

The slide features a blue background with a white atom symbol and a circuit-like pattern. A presenter in a pink shirt is visible in the bottom right corner. Logos for IIT Madras and NPTEL are in the bottom left.

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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**Chemical Reactor Design: General Procedure Outline**

**Step-1: Collect Required Data (Kinetic/Thermodynamic/Physical properties)**  
(Heat of reaction, Phase-equilibrium constants, Diffusion coefficients, Heat transfer coefficients, Mass transfer coefficients, etc)

The kinetic data required for reactor design will normally be obtained from laboratory and pilot plant studies. Values will be needed for the rate of reaction over a range of operating conditions: pressure, temperature, flow-rate and catalyst concentration.

Collect the physical property data required for the design; either from the literature, by estimation or, if necessary, by laboratory measurements.

The slide features a blue and white background with faint chemical symbols and icons. A presenter in a purple shirt is visible in the bottom right corner. Logos for institutions are visible in the bottom left corner.

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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## Chemical Reactor Design: General Procedure

### Step-2: Determine the Rate-limiting Step.

The reaction rate is usually limited by one of the following fundamental processes:

- Intrinsic kinetics (Rate of reaction itself)
- Mass-transfer rate (Important in multiphase reactions, porous catalyst)
- Heat-transfer rate
- Feed addition rate (control for highly exothermic/fast reaction)
- Mixing rate

The rate-limiting step can be determined experimentally by collecting rate data and fitting a suitable model of reaction kinetics.



Dr. Manoj Kumar



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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## Chemical Reactor Design: General Procedure

### Step-3: Select Reactor Type and Reaction Conditions

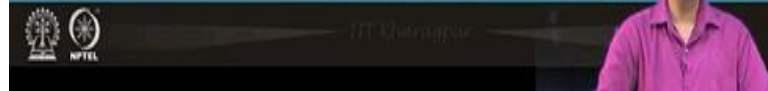
Choose a suitable reactor type, based on experience with similar reactions, or from the laboratory and pilot plant work. Make an initial selection of the reactor conditions to give the desired conversion and yield.

Reaction condition should optimize reactor conversion, yield, selectivity, should be safe, controllable, reasonable cost.

Reaction condition governs selection of reactor type – if reactants, products are all in vapour phase, CSTR will not be applicable.

### Step-4: Determine Materials of Construction

(Reaction condition – T, P, presence of particular component – will govern MOC)



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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## Chemical Reactor Design: General Procedure

### Step-5: Preliminary Sizing, Layout, and Costing of Reactor

Size the reactor. Exact analytical solutions of the design relationships may not always be available; semi-empirical methods based on the analysis of idealised reactors will normally have to be used.

The volume estimated is only the active reacting volume, and the reactor layout must also consider the following factors that may add to the volume required for the reactor vessel:

Additional space needed for (1) Any internal heat transfer devices such as coils, (2) Spargers for vapour-liquid distribution, (3) Inert vapour space in CSTR makes pressure control easier, (4) Catalyst support in packed bed or moving bed, (5) Fluid distribution grids, cyclones for fluidized bed reactor



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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## Chemical Reactor Design: General Procedure

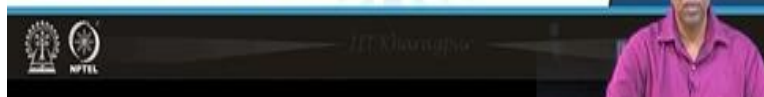
### Step-6: Estimate Reactor Performance

It is important to confirm that the reactor 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 (expensive option)

Historically, chemical companies would go through multiple steps of pilot-plant scale-up to validate their reactor designs. Nowadays, a more common approach is to use a combination of experimental methods and computer modelling to attempt to predict the full-scale performance.

### Step-7: Optimize the Design

### Step-8: Prepare Scale Drawings for Detailed Design



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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**Chemical Reactor Design: General Procedure**

In choosing the reactor conditions, particularly the conversion, and optimising the design, the interaction of the reactor design with the other process should also be considered.

The degree of conversion of raw materials in the reactor will determine the size, and cost, of any equipment needed to separate and recycle unreacted materials.

In these circumstances the reactor and associated equipment must be optimised as a unit.

The diagram illustrates a process flow starting with a 'Reactor Network' box. An arrow from this box points to a 'Product Separation' box. From the 'Product Separation' box, an arrow labeled 'Main Product' points to the right, and an arrow labeled 'Byproducts' points downwards. A feedback loop is shown with an arrow from the 'Product Separation' box going up to a 'Recycle Unit' box, which then has an arrow pointing back to the 'Reactor Network' box.

The slide also features the NPTEL logo in the bottom left corner and a small inset video of a man in a pink shirt in the bottom right corner.

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

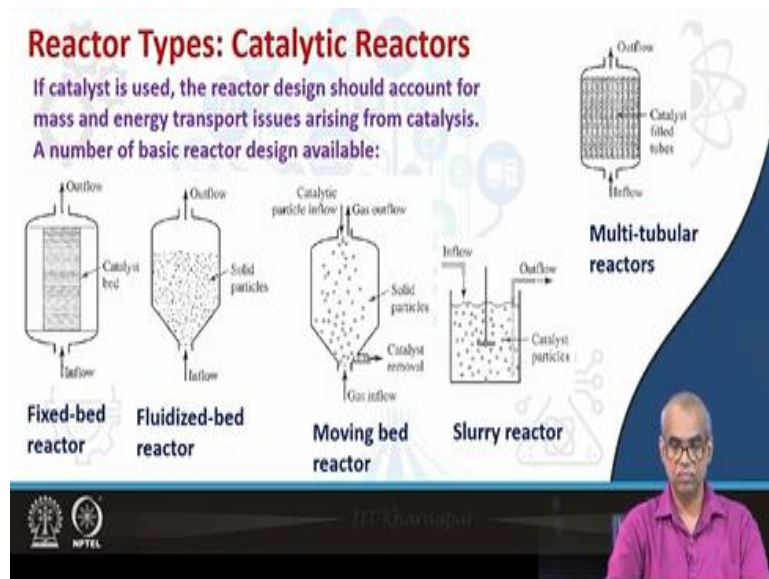
optimization of reactor separation system together, so we consider reactor separation system as one unit and then optimize the process.

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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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## Selection of Catalyst



Catalyst can reduce residence time requirements, provide greater selectivity for the desired product, and thereby reduce investment and operating costs.



There is no single path of finding a catalyst for a particular chemical reaction. It is both an art and a science. Experience, imagination, trial and error experimentation, and scientific analysis provide guidance for the selection.

Current Approach: Catalyst design guided by Molecular Dynamics Simulation.



Dr. Choudhary



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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### Reactor Types: Adiabatic Reactors

Adiabatic operation are preferred for simplicity of design. The reforming reactions are mostly endothermic. In adiabatic operation, the temperature would fall during the course of the reaction. If the reactor were made as one single unit, this temperature fall would be too large. Either high inlet  $T \Rightarrow$  undesired reactions Or low outlet  $T \Rightarrow$  incomplete reaction. The problem is conveniently solved by dividing the reactor into three sections. Heat is supplied externally between the sections.

Reactor section for the catalytic reforming of petroleum naphtha (for improving the octane number of gasoline)

Reactants

Reactor charge furnace

Reactor

Intermediate furnace

Products

NPTEL

Dr. Choudhary

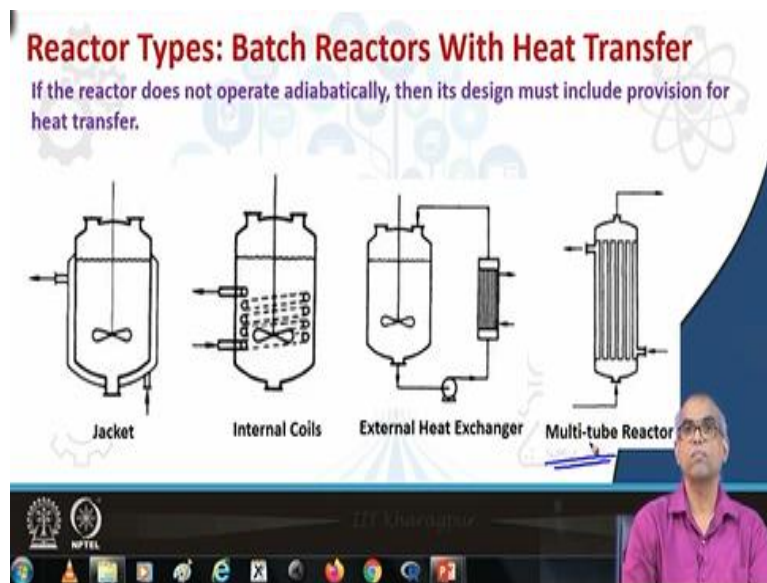
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What you see in figure is the reactor section for the catalytic reforming of petroleum naphtha, the reforming of petroleum naphtha is done for improving the octane number of the gasoline. Adiabatic operations are preferred for simplicity of design. 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 its 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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## Selection of Reactors: Heuristics

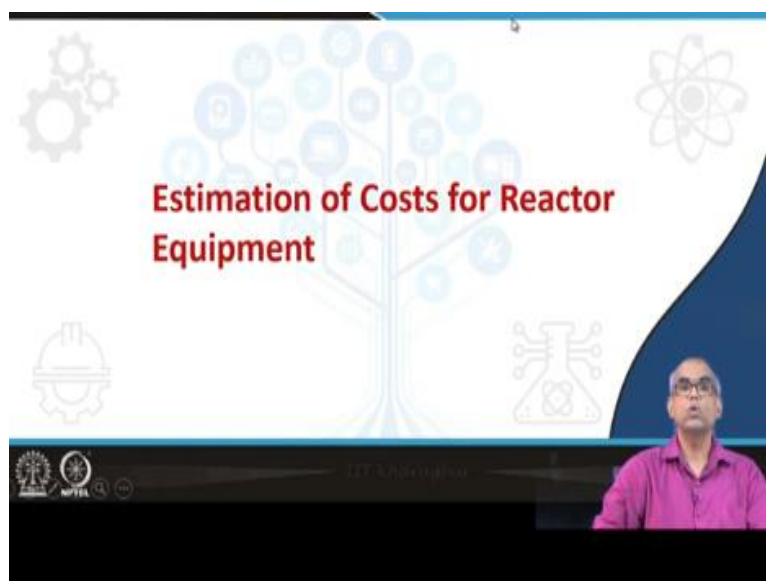
1. For conversions up to 95% of equilibrium the performance of five or more CSTRs connected in series approaches that of a PFR.
2. CSTRs are usually used for slow liquid-phase or slurry reactions.
3. Batch reactors are best suited for small-scale production, very slow reactions, those which foul, or those requiring intensive monitoring or control.
4. The typical size of catalytic particles is approximately 0.003 m for fixed-bed reactors, 0.001 m for slurry reactors, and 0.0001 m for fluidized-bed reactors.
5. Larger pores in catalytic particles favour faster, lower-order reactions; conversely, smaller pores favour slower, higher-order reactions.



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.

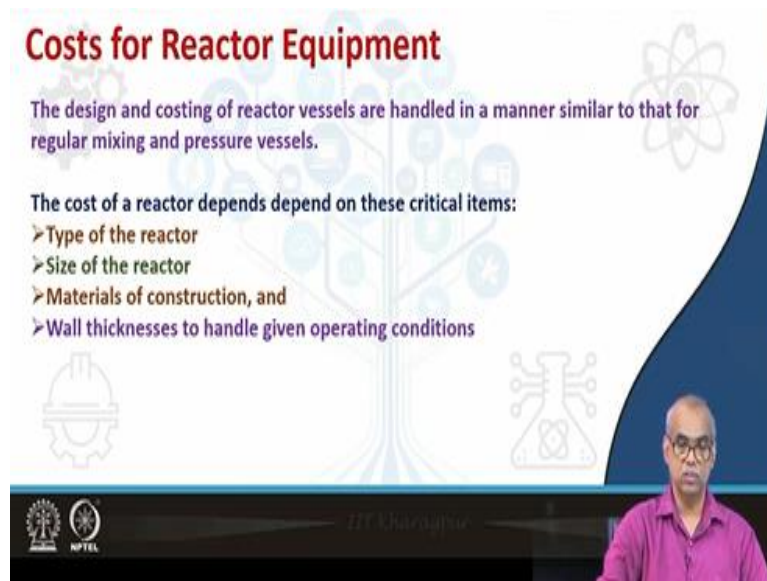
The typical size of catalytic particles is approximately 0.003 meter for fixed-bed reactors, 0.001 meter for slurry reactors and 0.0001 meter for fluidized bed reactors. Large pores in catalytic particles, favour faster, lower-order reactions conversely, smaller pores favour slower, higher-order reactions. 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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**Costs for Reactor Equipment**

The design and costing of reactor vessels are handled in a manner similar to that for regular mixing and pressure vessels.

The cost of a reactor depends on these critical items:

- Type of the reactor
- Size of the reactor
- Materials of construction, and
- Wall thicknesses to handle given operating conditions

The slide features a background with faint icons of a reactor, a tree, and a molecular structure. The presenter is a man in a purple shirt, visible in the bottom right corner. Logos for IIT Madras and NPTEL are in the bottom left.

The design and costing of 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 given 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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**Costs for Reactor Equipment**

Many reactors are designed to be operated at high pressures and such reaction vessels are classified as pressure vessels.

Once the reactor dimensions have been determined, the pressure vessel design methods can be used to estimate the wall thickness and hence determine the capital cost.

Additional costs may need to be added to cover the cost of reactor internals or other ancillary equipment such as agitators.

The slide features a background with faint icons of a reactor, a tree, and a molecular structure. The presenter is a man in a purple shirt, visible in the bottom right corner. Logos for IIT Madras and NPTEL are in the bottom left.

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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### Costs for Reactor Equipment: Thickness

Minimum Wall Thickness for Pressure Vessels: Cylindrical Shells

**Limiting Condition**

$$t = \frac{Pr_i}{SE_j - 0.6P} + C_c$$

$\left\{ \begin{array}{l} t \leq \frac{r_i}{2} \\ \text{or } P \leq 0.385SE_j \end{array} \right.$


**Limiting Condition**

$$t = r_i \left( \frac{SE_j + P}{SE_j - P} \right)^{1/2} - r_i + C_c$$

$\left\{ \begin{array}{l} t > \frac{r_i}{2} \\ \text{or } P > 0.385SE_j \end{array} \right.$

*> Peters, Timmerhaus, West  
> Pressure vessel code*

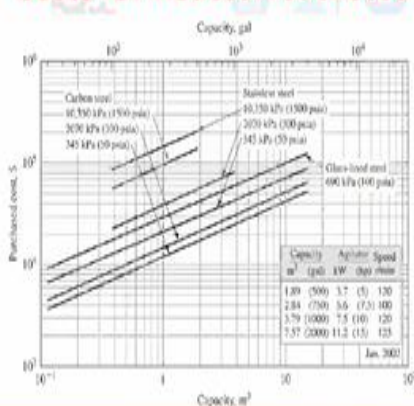
**Legend:**  
 $t$  = minimum wall thickness, m  
 $P$  = maximum allowable internal pressure, kPa (gauge)  
 $r_i$  = inside radius of shell, before corrosion allowance is added, m  
 $S$  = maximum allowable working stress, kPa  
 $E_j$  = efficiency of joints expressed as a fraction  
 $C_c$  = allowance for corrosion, m



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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### Costs for Reactor: Jacketed Stirred Tank Reactor



**The costs of jacketed stirred-tank reactors are not addressed using simple pressure vessel cost correlations alone.**

**A substantial part of the cost is in the construction of the vessel jacket.**

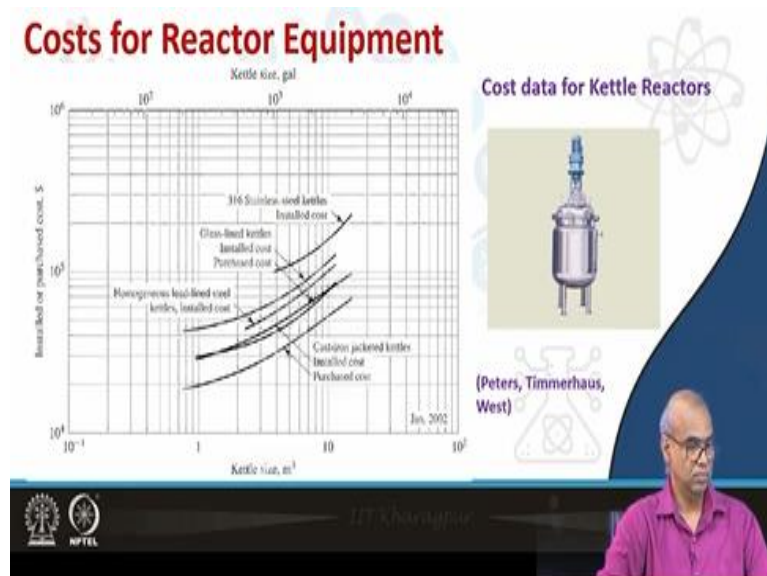
*(Peters, Timmerhaus, West)*



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.

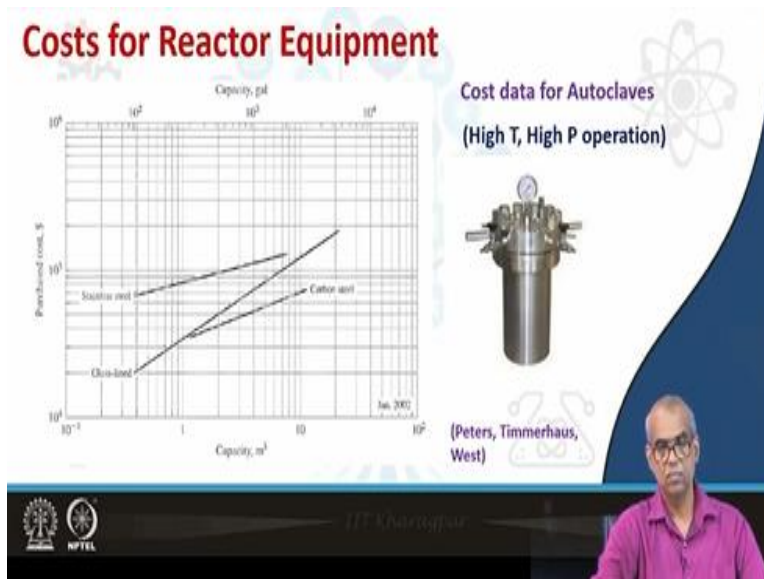
So, such graphical correlations can be used to find out the purchase cost given particular capacity and operating conditions and materials constructions, note that both for carbon steel and stainless steel the data are given for various pressures; 50 psi, 300 psi and 1500 psi. So, such graphical correlations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

Consider design of a cylindrical reactor. Let there is no internal accessory (cooling/heating coils)

1. Find dimensions of the reactor (Length, Diameter, Thickness)
2. Find weight of shell ( $W_s$ )
3. Select head of vessel: Hemispherical/Ellisoidal/Torispherical
4. Find weight of two heads ( $W_h$ )
5. Find weight of shell + head,  $W_{sh} = W_s + W_h$
6. Find total weight ( $W_T$ ) by adding 15% to ( $W_s + W_h$ ) for nozzle, manhole, saddle, etc.  $W_T = 1.15(W_s + W_h)$

Use available cost correlations for preliminary cost estimation.

If MOC is Carbon Steel: Cost per kg of fabricated unit =  $73(W_T)^{-0.34}$

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.