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

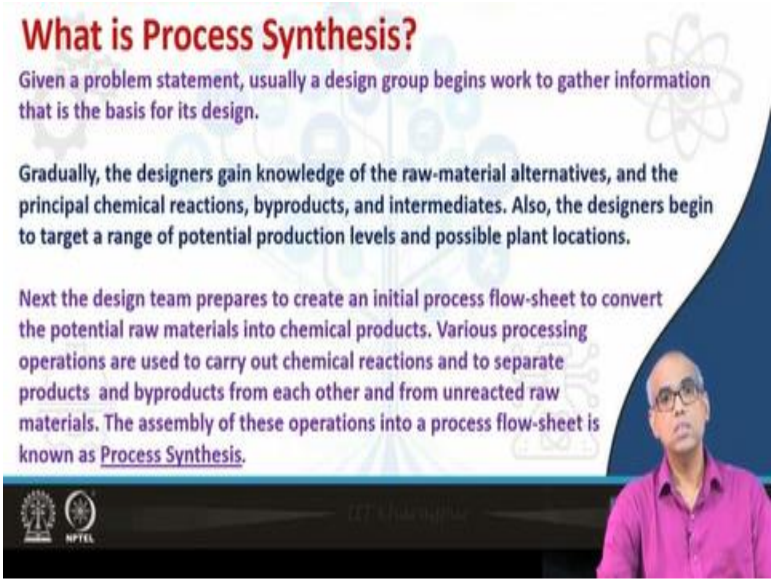
**Lecture No -26**
**Introduction to process Synthesis**

Welcome to the lecture 26 of plant design and economics, in this module we will talk about conceptual process synthesis. When we produce a target product in an industrial scale operation the process operations will involve series of operations, series of processing units. Now process synthesis means that we have select appropriate process units we have to put them together in appropriate sequence and we have to established a very efficient inter-connection among these units.

So the ultimate goal is to get and efficient process flow sheet which will production of the desired product in an economic and safer manner. Note that the operation has to be economically attractive as well as it has to be safe to humans as well as environments. So in this module we will learn about how to conceptually synthesize chemical processes, broadly speaking there are two main ways of achieving this goal.

One is known as hierarchical approach to process synthesis, another is algorithmic approach to processes synthesis. Hierarchical approach depends on the past knowledge of the scientists and engineers working in this area and algorithmic approach involve mathematical optimization techniques. We will mostly focus our attention on hierarchical approach to process synthesis.

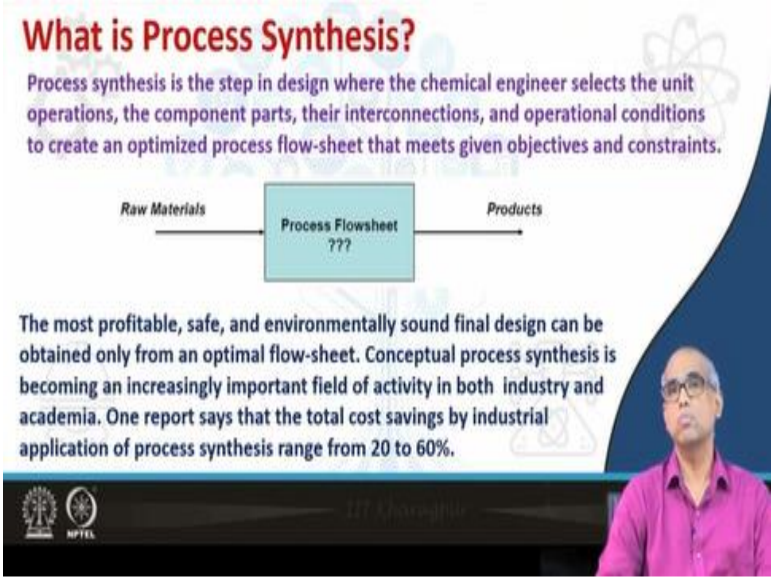
**(Refer Slide Time: 02:10)**




So today's lecture will be based on introduction to process synthesis, we will define various terms that will be frequently using throughout the module. Now let us first try to understand more detail what exactly is process synthesis? Given a problem statement, usually a design group begins together information that is the basis of it is design. Gradually the designers gain knowledge of the raw material alternatives, and the principle chemical reactions, byproducts, and intermediates.

Also the designers begin to target a range of potential production levels, and possible plant locations. Next the design team prepares to create an initial process flow sheet to convert the potential raw materials into chemical products. Various processing operations are used to carry out chemical reactions and to separate products and by products from each other and from un-reacted raw materials. The assembly of these operations into a process flow sheet is known as process synthesis.

**(Refer Slide Time: 03:44)**

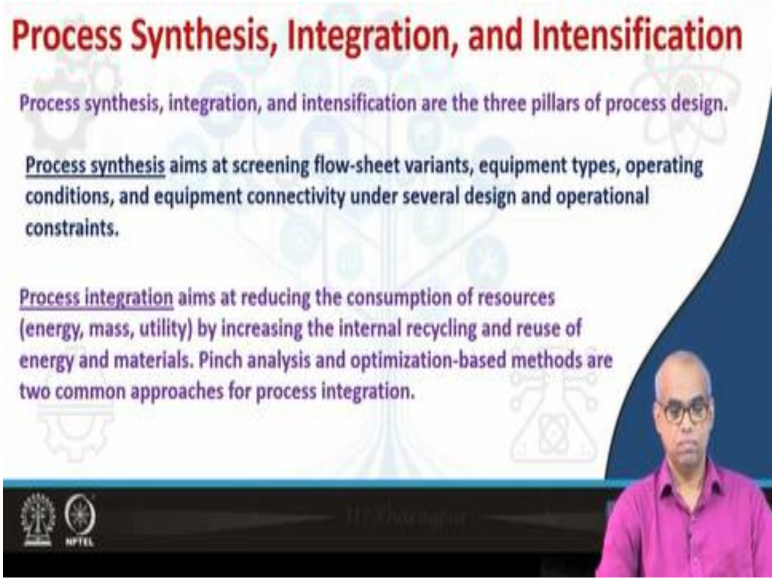



So process synthesis is the step in design where the chemical engineer selects the unit operations, the component parts, their inter-connections and operational conditions to create an optimized process flow sheet that meets given objectives and constraints. The objectives will generally be associated with your target products it is production levels etcetera. Constraints come in various ways, there will be constraints related to operations, there will be constraints related to environmental and safety requirements.

So if you look at the block diagram, the raw material goes to the black box and the products come out from the black box. So in the black box we have the process flow sheets and there will be various possible process flow sheets, we have to find the best alternative for the process. The most profitable, safe and environmentally sound final design can be obtained only from an optimal flow sheet.

Conceptual process synthesis is becoming an increasingly important field of activity in both industry and as well as in academia. For last few years in academic research also the process synthesis has gained tremendous popularity. One report says that the total cost savings by industrial application of process synthesis range from 20 to 60%. So that is the big motivation for industry to adapt process synthesis in the very early stage of the design.

**(Refer Slide Time: 06:03)**

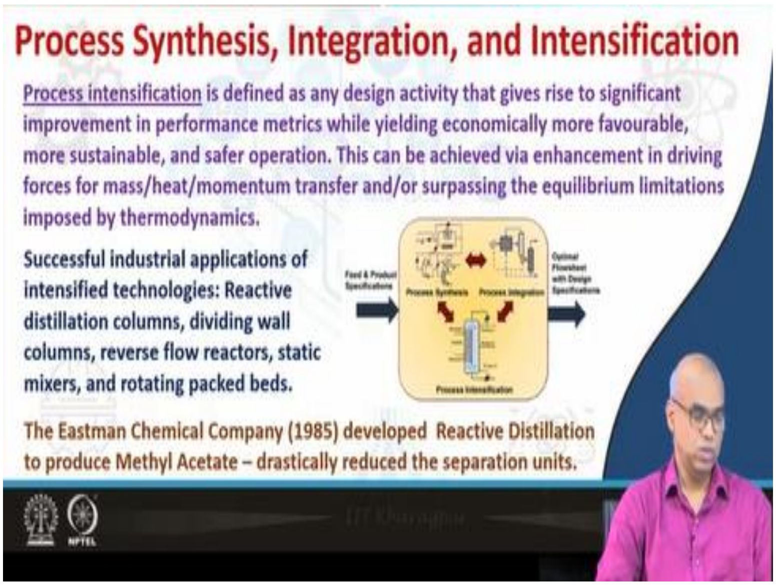



Now we will define three terms or two additional terms along with process synthesis: process synthesis, process integration and process intensification. Process synthesis, process integration, and intensification are the three pillars of modern process design. Process synthesis aims at screening flow sheet variants, equipment types, operating conditions and equipment connectivity under several design and operational constraints.

Process integration aims at reducing the consumption of resources such as energy, mass, utility by increasing internal recycling and reuse of energy and materials. Pinch analysis and optimization based methods are two common approaches for process integration. The two common commodities that are consumed in any chemical process industry are energy and mass.

So both energy integration and mass integration are very important for a chemical process industry these leads to an efficient and sustainable process. So wherever it is possible we must try to recover heat or recover energy by adopting appropriate energy integration or heat integration strategy, the same holds true for mass integration.

**(Refer Slide Time: 08:08)**

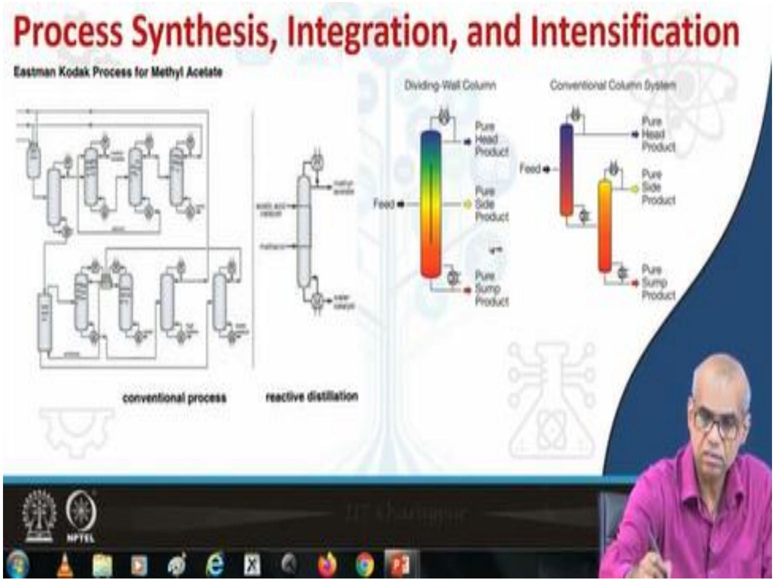



Process intensification is defined as any design activity that gives rise to significant improvement in performance metrics while yielding economically more favourable, more sustainable and safer operation. This can be achieved by an enhancement in driving forces for mass transfer, heat transfer, and momentum transfer and or surpassing the equilibrium limitations imposed by thermodynamics.

So you can see in the cartoon, how this process synthesis, process integration and process intensifications are interconnected to for obtaining the most efficient flow sheet that converts the raw materials into finished products. There are several successful industrial applications of intensified technologies, some examples are reactive distillation columns, dividing wall columns, reverse flow reactors, static mixers and rotating packed beds.

The Eastman chemical company 1985, developed reactive distillation to produce Methyl Acetate, the conventional production of Methyl Acetate used several distillation columns as separation systems, whereas the Eastman chemical company's reactive distillation strategy drastically reduced the separation units.

**(Refer Slide Time: 10:10)**



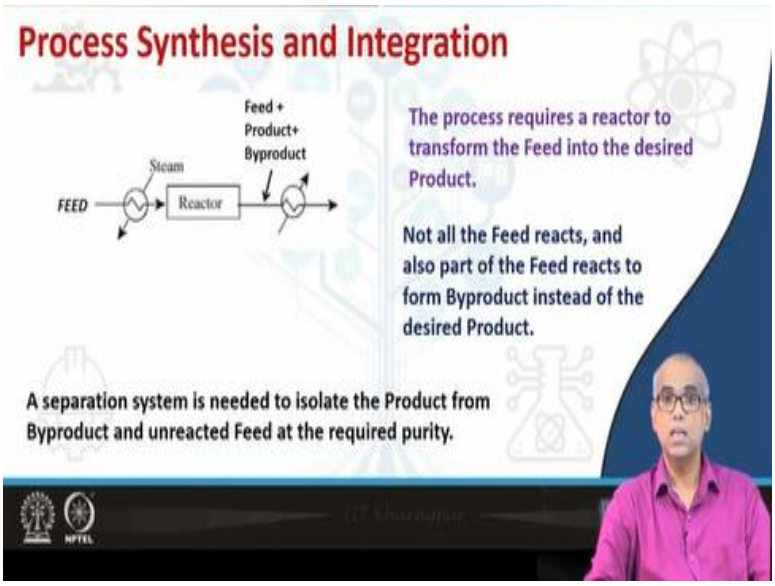

It will be clear if you look at this diagram, what you see here? Is the conventional process for production of Methyl Acetate, you can see that there is a series of distillation columns for separation of the products and un-reacted feeds etcetera. In case of reactive distillation you obtained the Methyl Acetate which can obtain by reacting Acetic acid with methanol in presence of catalyst.

Now this operation can be carried out in a distillation column, so the same equipment or processing unit is serving the purpose of the reactor as well as separator, this drastically reduces the number of processing states or processing units, thereby process is being intensified. Same holds true for dividing column, or dividing wall column, distillation unit. Suppose we are separating a three component mixture A, B, C.

So, you have to separate components A, B and C, in conventional columns you require two distillation columns to separate A, B and C. What you can do is? Let us say I first take out A from the top of the first distillation column and the bottom product contains B and C. So B and C is being feed to the second distillation column and B comes from the top of the second distillation column and C comes from bottom of the second distillation column.

But in case of dividing wall column you are putting a wall within the distillation column and then it is possible to separate all three components from the same distillation column. Again this is leading to process intensification.

**(Refer Slide Time: 13:04)**



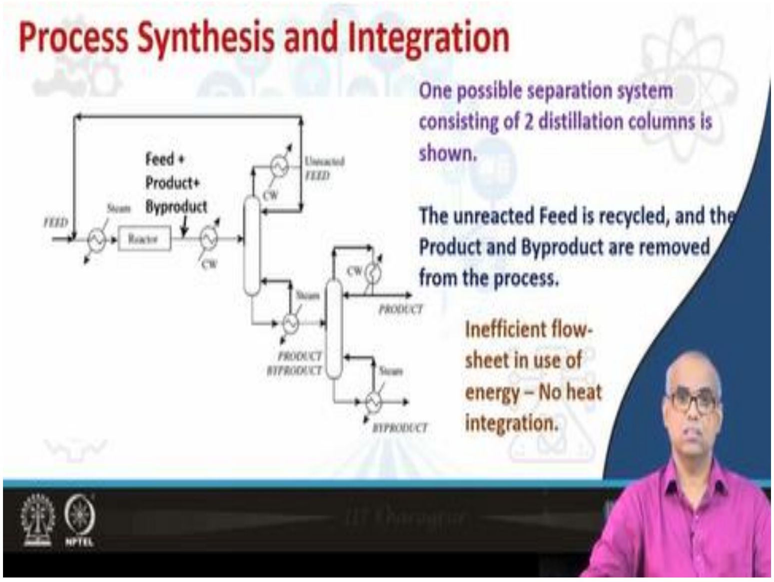

Now, let us look at this process synthesis and integration in slightly more detailed. Look at the flow sheet, the process uses a reactor to transform the feed into desired product but it is may not be possible to convert all the feed into the desired product. So there will be some un-reacted feed, in the effluent stream there will also be some byproduct. So the effluent stream that comes of the reactor will contain feed the desired product as well as it may also contains a byproduct.

So, what do we do next? Obviously a separation system will be required to separate the product, the desired product from the by product and un-reacted feed. So, we understand that after the reactor we have to place a separation unit or a separation system, one separation unit may not be enough. For example, A single distillation column may not be enough to separate this feeds, products and by products.

So it may be possible that you have to use a separation train or a sequence of distillation column for a specific example. Idea is that the effluence feed for reactor contains feed, by product and product; so to separate this desired product from feed and by product, I must now use a separation unit. So putting a separation unit of the reactor in a separator will be logical step to take.

Now let us say the separator is able to separate the products from the feed and the by product. So what we will do in this feed? The feed can be sent back to the reactor as a recycled strip. So the separator and the recycled stream will follow the reactor, so this is what we can logically conclude.

**(Refer Slide Time: 16:21)**



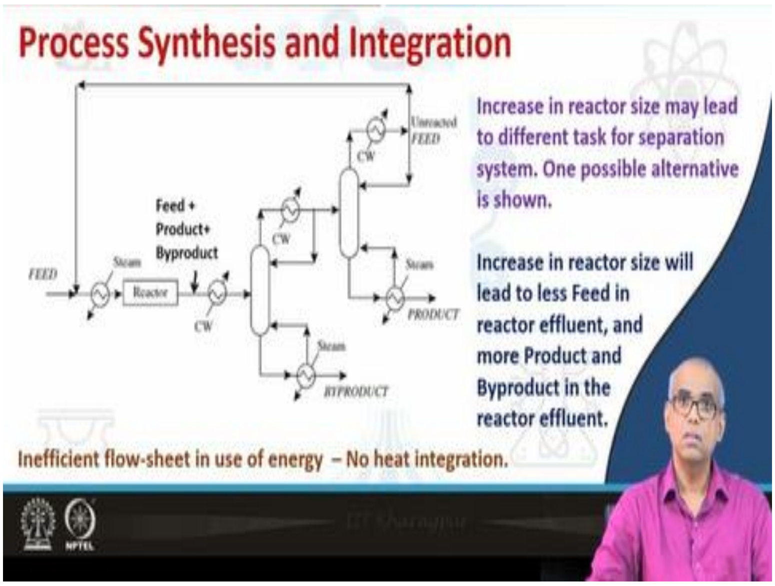

So one possible separation system consisting of two distillation columns is shown in the flow sheet, note that there are many several possible alternatives; it is not the only alternative that is possible. So you can think of various possible separation systems to separate the feed product and the by product. The example that is shown here consists of two distillation columns.

Look at the first distillation column, the first distillation column takes feed product and by product mixture as feed and from the top of the distillation column the feed is un-reacted feed is obtained and from the bottom of the first distillation column mixture of product and by product is obtained. These un-reacted feed is the recycle to the reactor, so it mixes with the feed and note that there is a heat exchanger because it may be possible to take the feed stream to an appropriate temperature to heat up before entering the reactor.

Similarly, the effluent stream from the reactor is cooled down using a heat exchanger before it enters the distillation column, so such heat exchanges will be required. Now come to the second distillation column, the second distillation columns takes the by product and the product mixture as feed and it is separates this mixture into a stream of product and by product which comes from the top and bottom of the distillation column respectively.

So the un-reacted feed is recycle to the reactor before entering the reactor it mixes with the feed, so that it can be preheated and the product and by products are removed from the process. So this is one possible flow sheet, now this flow sheet is inefficient in terms of use of energy because you see that there is no heat integration, no attempt has been made to recover heat.

**(Refer Slide Time: 19:56)**



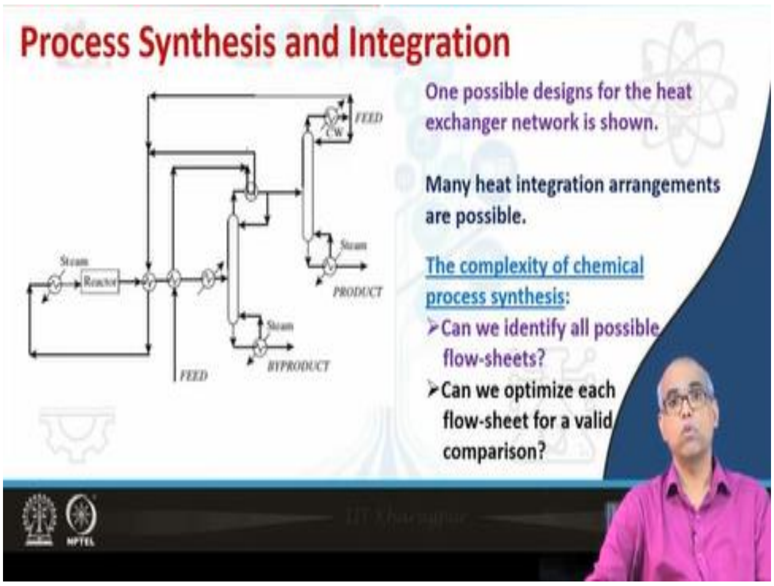

Now let us consider that, now I increase the reactor size, so if we use a reactor of different size this will lead to different task for separation system, why? Because when you increase the reactor size, there may be less feed in the effluent from the reactor but there will be more products and by product, so more amount of feed is getting converted to product and by product.

So the effluent stream now contains less of feed or less of un-reacted feed and more of product and by product, so this may lead to different task for separation system and this scenario we may be interested to separate product and by product first. So how you do that? you are effluence stream from the reactor is a mixture of less amount of feed and more amount of product and more amount of by product.

So this goes to the distillation column 1 and I separate this into a mixture of un-reacted feed and product which comes from the top of the distillation column and by products stream which comes from bottom of the distillation column, then this un-reacted feed and the product stream goes to the distillation column number 2, which separates this mixture into stream of un-reacted feed and stream of desired product.

Again, the un-reacted feed goes as the recycle stream mixes with the feed preheated and enters the reactor. So this is again one possible alternative there may be other alternatives as well. Again, this flow sheet is also inefficient in terms of energy uses because of the same reason no attempt has been made to recover energy and heat integration.

**(Refer Slide Time: 22:50)**




So this flow sheet shows one possible design for the heat exchanger network, so here attempt has been made to recover energy or recover heat. Note that, the feed enters from here exchanges heat with the effluence stream, so gets preheated. It also exchanges heat with the vapour stream that comes out from the top of the distillation column, so attempt has been made to recover energy from the available streams in the process.

Note that there will be many integration arrangements and this is just one possible design. Later on we will talk about this energy recovery in more detail, so whatever we have seen so far, what are the complexities of chemical process synthesis? Whatever you have discussed so far on the basis of that we can say that the complexity are mainly two flow sheets. One, can you identify all possible flow sheets, is it possible to identify all possible flow sheets?

See by inspection can you identified all possible flow sheets, is it possible to imagine the every possible way the instruments can be interconnected, can you also optimize each flow sheet for a valid comparison? So before we compare to flow sheets, we must optimize to the extent possible both the flow sheets, then only it becomes a valid comparison. So these two we choose leads to great complexity for chemical process synthesis.

Can you identify all possible flow sheets? Can you optimize each flow sheet for a valid comparison?

**(Refer Slide Time: 25:35)**

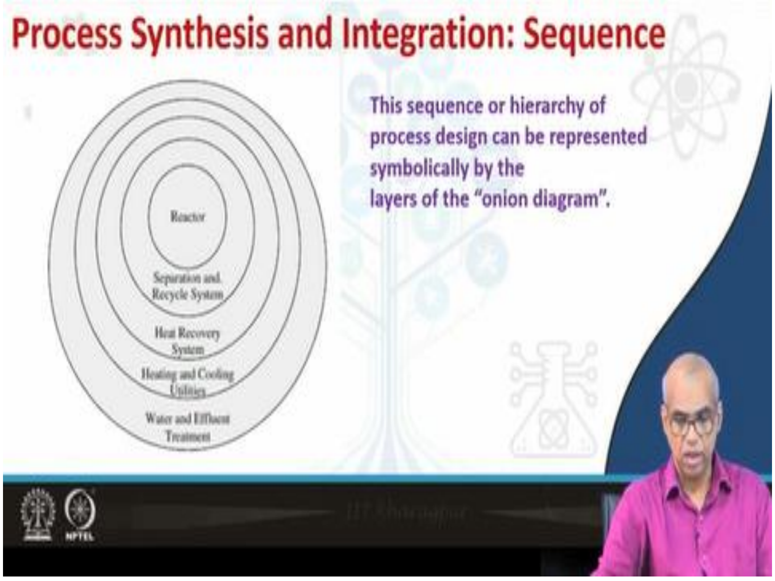

Now, let us look at the sequences of chemical conceptual process synthesis and integration, if raw materials are converted into products that design will usually start with the design of the reactor, you may have some processes where you do not have a reaction. Let us say your process consists of separation, so does not have a reactor; so the design may start with the separator, but whenever your raw materials to be converted into desired products the design will usually start with the reactor.

The chosen reactor design produces a mixture of un-reacted feed materials, products, and byproducts. Thus, the design of separation and recycle system will follow, this is what we have seen when we talked about the possible flow sheets in first few slides. So note that the reactor that you have chosen will determine the separation and recycle system. The reactor and separation and recycle system designs together will define the heating and cooling duties for your process.

So obviously the design of heat exchanger network will come next. Now it is not possible to use energy, the entire energy that is required for your process from the recovered energy. Heat integration will of course will lead to sustainable design will add to your process economics, but it is not possible that we will meet the entire energy requirement from the recover energy. So design of utility system will always be required.

So, energy needs to be used from utility resources, so design of utility systems will be considered after we have considered the heat exchanger network. Note that different processes in your plant may be connected to the same utility system, so this is next to some complexity in the design of the utility system. Finally, you are discharge from the plant must meet the environmental requirement and we consider finally the design of water and effluent treatment system.

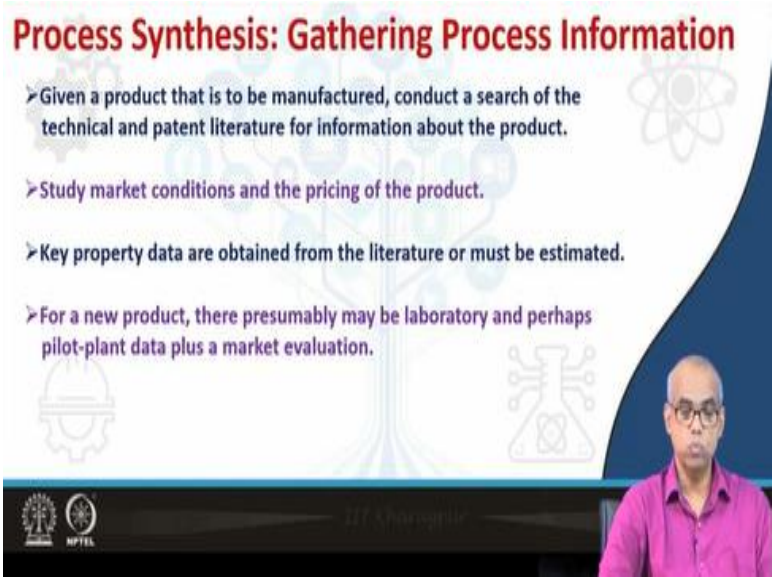
**(Refer Slide Time: 29:26)**




So this sequence of a process design can be represented symbolically by the layers of what is known as onion diagram. This sequence of process design is also known as hierarchy of a process design. So this is symbolically represented by the layers of onion diagram, so the innermost layer is the design of the reactor. Next layer separation and recycle system, next, heat recovery system or energy integration.

Then utility systems, heating utility as well as cooling utility and finally water and effluent treatment. So this onion diagram symbolically represents the sequence of hierarchy of process design.

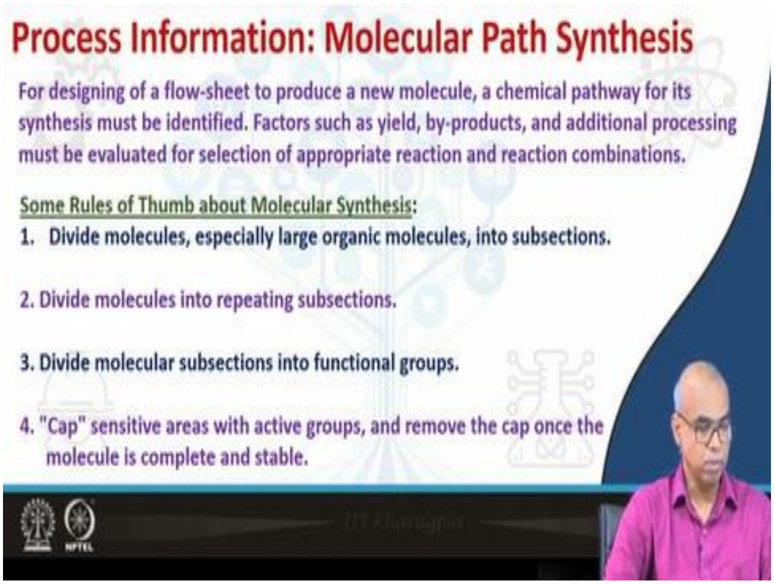
**(Refer Slide Time: 30:32)**




Now, the process synthesis will normally start with the gathering process information; you must gather information about your process. Given a product that is to be manufactured, we have to conduct a search of the technical and patent literature for information about the product. Study market conditions and the pricing of the product, key property data are obtained from the literature or must be estimated.

For a new product there may be laboratory and perhaps pilot plant data plus a market evaluation. So this may be required for a new product.

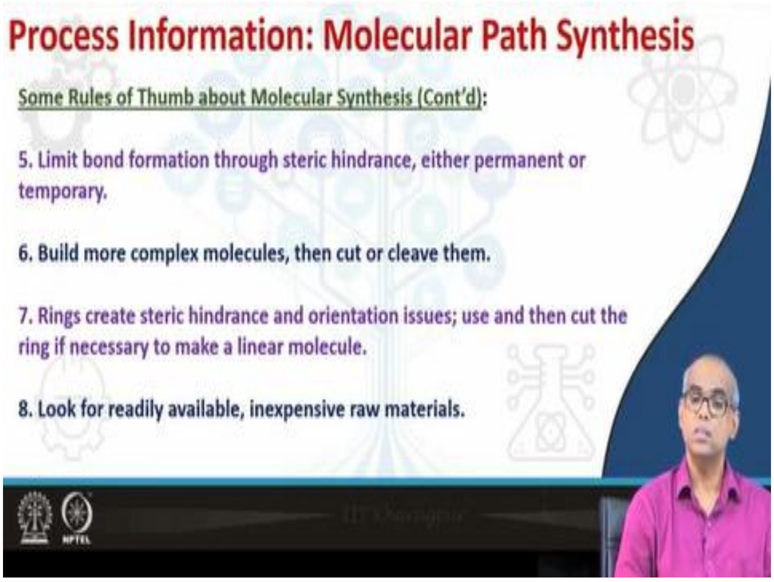
**(Refer Slide Time: 31:25)**




Whenever you are designing a flow sheet for production of a new molecule, a chemical pathway for its synthesis must be identified. So molecular path synthesis will be required when my target product is a new molecule, factor such as yield, by products and additional processing must be evaluated for selection of appropriate reaction and reaction combinations. Here are some rule of thumb about molecular synthesis; divide molecules, especially large organic molecules into subsections.

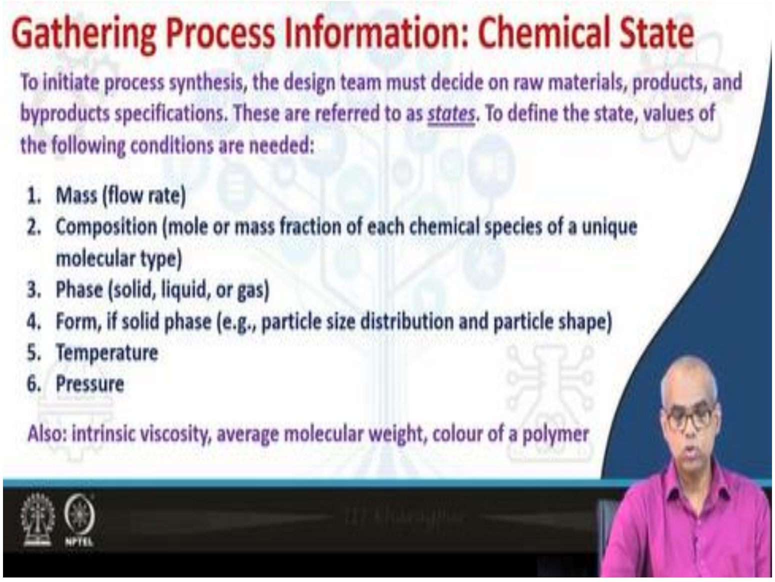
Divide molecules into repeating subsections, divide molecular subsections into functional groups. Cap sensitive areas with active groups, and remove the cap once the molecule is complete and stable.

**(Refer Slide Time: 32:33)**




Limit bond formation through steric hindrance, either permanent or temporary. Build more complex molecules, then cut them or cleave them. Rings create steric hindrance and orientation issues; use and then cut the ring if necessary to make a linear molecule. Look for readily available, inexpensive raw materials. So, these are some rules of thumb for molecular synthesis.

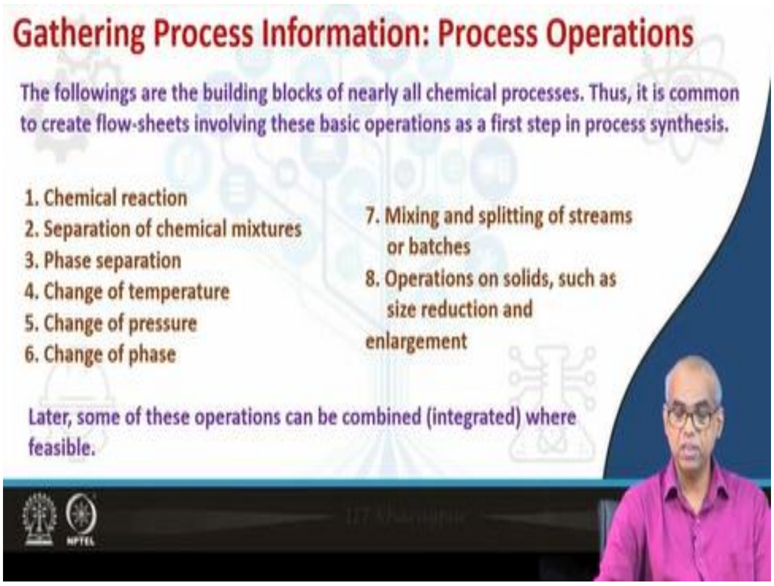
**(Refer Slide Time: 33:18)**




Now, there are other information's about the process that must be gathered; chemical state. To initiate process synthesis, the design team must decide on raw materials, products, and by products specifications; these are referred to as states. To define the states, values of certain conditions are needed; the following are those conditions: Mass, Composition, Phase, solid, liquid or gas. Form, if solid phase; such as particle size distribution and particle shape, etcetera temperature and pressure.

So define state values for these conditions are needed. Also, intrinsic viscosity, average molecular weight, colour of a polymer may also be required.

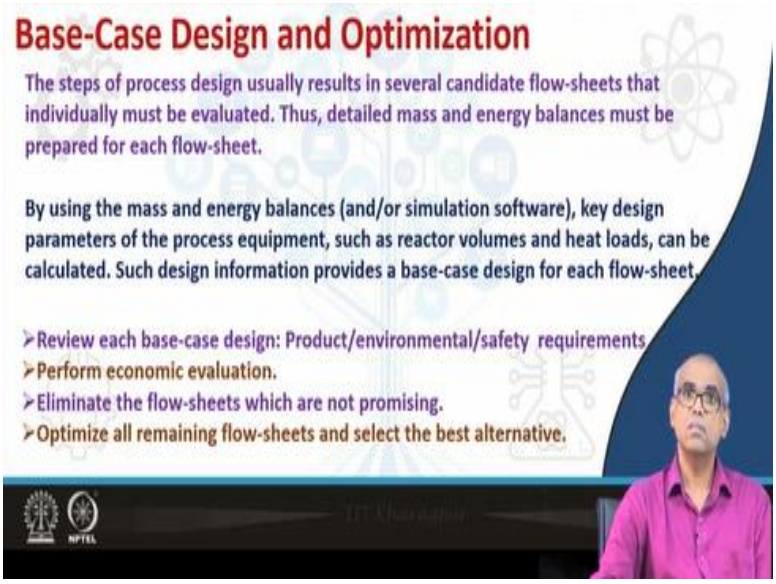
**(Refer Slide Time: 34:37)**




Then you must gather information about process informations; you are familiar with various unit operations. Now, we list certain operations which are like building blocks of nearly all chemical processes. For example, chemical reactions, separation of chemical mixtures, phase separation, change of temperature, change of pressure, change of phase. Mixing and splitting of strings or batches, operations on solids, such as size reduction and enlargement.

So these operations are building blocks for nearly all chemical processes, you see such operation in various chemical processes. Thus it is common to create flow sheets involving these basic operations as a first step in process synthesis. Later on, some of these operations can be combined that means can be integrated where feasible, which will lead to process integration as well as process intensification.

**(Refer Slide Time: 36:09)**

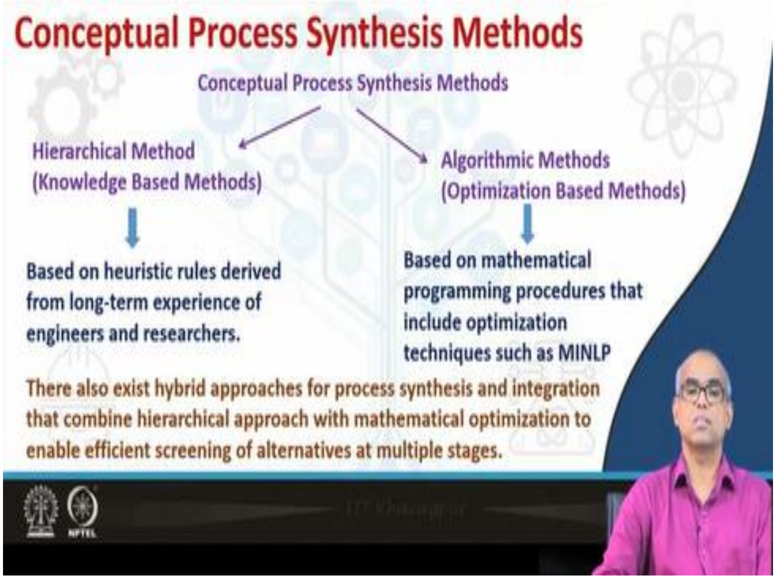



Now, let us look at the process synthesis as a whole in very brief. The steps of process design usually results in several candidate flow sheets that individually must be evaluated. So you will follow certain process design steps or synthesis steps and this will lead to several candidate flow sheets and you must evaluate the merits of such flow sheets individually. Thus detailed mass balance and energy balance are required for each flow sheet.

By using the mass energy balances and all use of simulation software, key design parameters of the process equipment such as reactor volumes and heat loads can be calculated, such design information provides a base case design for each flow sheet. Now we should review each base case design you must ensure whether this designs meet product specification, environmental requirement, safety requirement, health standards, etcetera.

We must perform economic evaluations on these base case designs on the basis of these we should be able to eliminate those flow sheets that are not promising. Before eliminating you can see whether some adjustments of the conditions can make them promising or not, after eliminations of the non-promising flow sheets, we should optimize the remaining flow sheets and select the best alternative. So that is in a nutshell, we will now talk about in more details in future classes.

**(Refer Slide Time: 38:43)**




Now this step of the conceptual process synthesis of the methods of the conceptual process synthesis can be broadly classified into two categories: hierarchical methods known as knowledge based methods and algorithmic method which are based on mathematical optimization techniques. The knowledge based methods depends on heuristic rules and these heuristic rules are derived from long term experience of engineers and researchers.

Whereas algorithmic methods are based on mathematical programming that includes optimization techniques, such as mixed integer nonlinear programming, etcetera. There also exist hybrid approaches for process synthesis as well as process integration, hybrid approaches combine both hierarchical approach that means knowledge based approach and mathematical optimization techniques or algorithmic methods to produce efficient screening of alternatives at multiple stages. With this we stop our discussion or introduction of conceptual process synthesis here.