Plant Design and Economics
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Lecture No -27
Hierarchical Approach to Process Synthesis -I

Welcome to lecture 27 of plant design and economics. In this is module we are talking about conceptual process synthesis. Now, the methods for conceptual process synthesis can be broadly classified into two categories one is hierarchical approach for process synthesis, another is algorithmic approach for process synthesis. In this module, we will mostly focus on hierarchical approach to process synthesis and very briefly talk about the algorithmic methods for process synthesis. So today we will start with part one of hierarchical approach to process synthesis.

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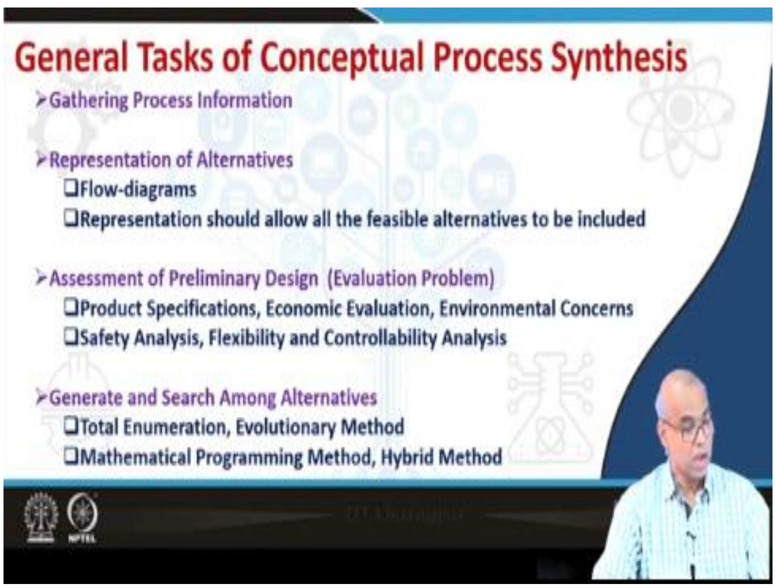

Now there are certain general tasks of conceptual process synthesis. First task is to gather process information. In our previous lecture, we have talked about what are the kinds of information that you must gather for the purpose of design. Second; representation of flow sheet alternatives or representation of process alternatives. These representations are done in terms of flow diagrams, our representation should allow all the feasible alternatives to be included and it will be better if the representation is smart enough to exclude the flow sheets that are not feasible.

Assessment of preliminary design: So this is essentially evaluation of preliminary design. The preliminary designs needs to be evaluated on the basis of product specification, economic evaluations, environmental concerns, safety analysis, flexibility as well as controllability analysis. The controllability analysis refers to the thing that whether the process is easily controllable or not, whether the flexibility refers to the fact that whether your process is flexible enough to accommodate any changes in the process.

Then generate and search among alternatives. So while selecting the best possible design, we must be able to generate various alternatives and search among the alternatives. There are various methods such as total enumeration, evolutionary methods, mathematical programming method, hybrid methods etcetera.

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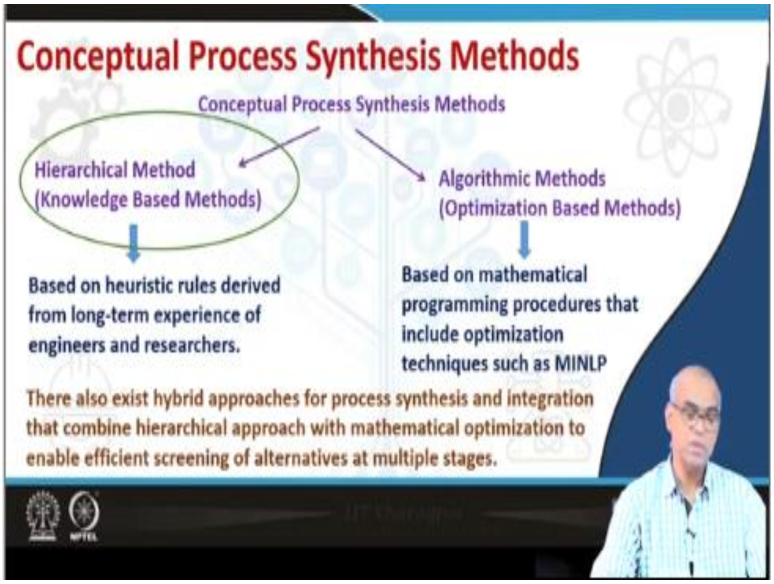

So as we discussed that conceptual process synthesis methods are broadly classified as hierarchical method and algorithmic methods. Hierarchical methods are essentially knowledge based methods. So they are based on heuristic rules derived from long term experience of engineers and researchers. Algorithmic methods are based on optimization techniques. So they are based on mathematical programming procedures that include optimization techniques such as mixed integer linear programming on mixed integer non-linear programming methods.

There also exist hybrid approaches for process synthesis as well as for process integration that combine hierarchical approach with mathematical optimization to enable efficient screening of alternatives at various Stages during the flow sheet development. In this module we will talk about hierarchical method in detail and very briefly outline the algorithmic methods. So we will mostly focus on hierarchical method or knowledge base method.

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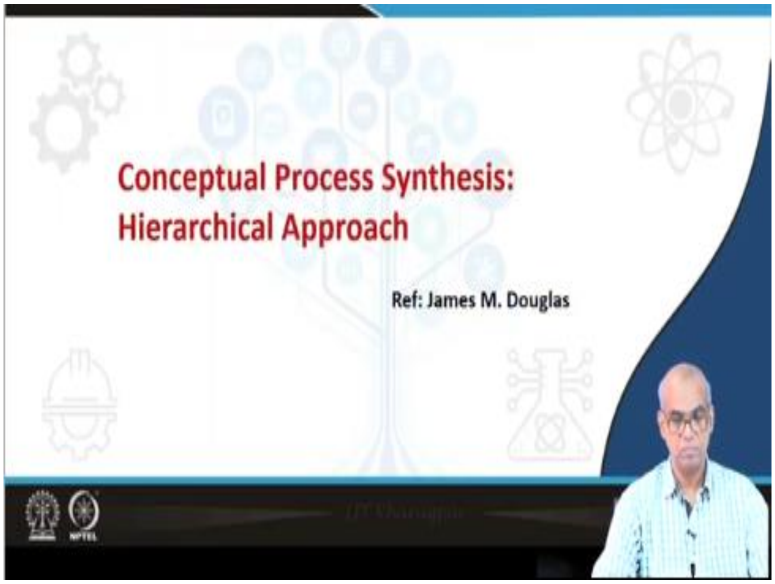

The conceptual process synthesis through hierarchical approach that will discuss here is taken from James M. Douglas.

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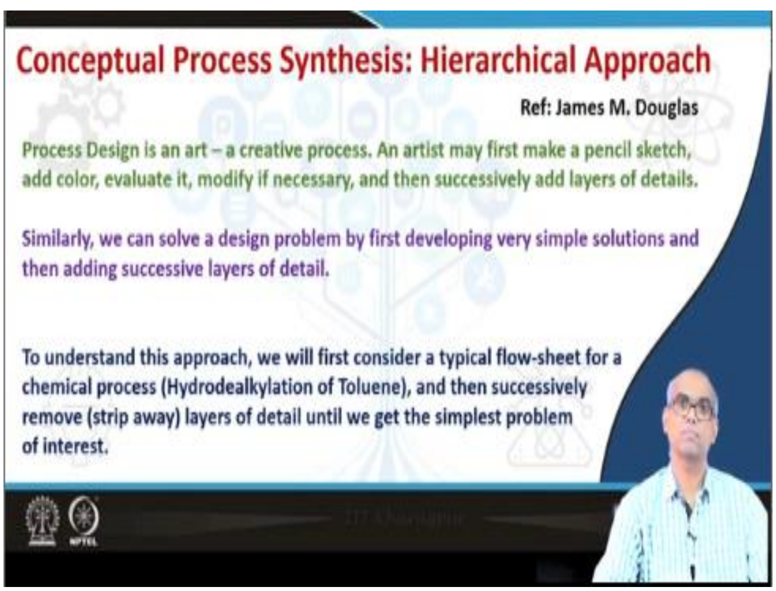

Process design is an art, it is a creative process. Think how an artist makes his or her painting. The artist may first make a pencil sketch, when the artist essentially focus on the key aspects of the painting and then add colours, evaluate it at various stages, modify if necessary and then successively add layers of details to the paintings and finally becomes a beautiful painting. Similarly we can solve a design problem by first developing a very simple solution and then go on adding successive layers of detail about the design.

To understand this approach, we will first consider a typical flow sheet for a chemical process in particular will take hydrodealkylation of Toluene and then successively remove or strip away layers of detail until we get the simplest problem of interest.

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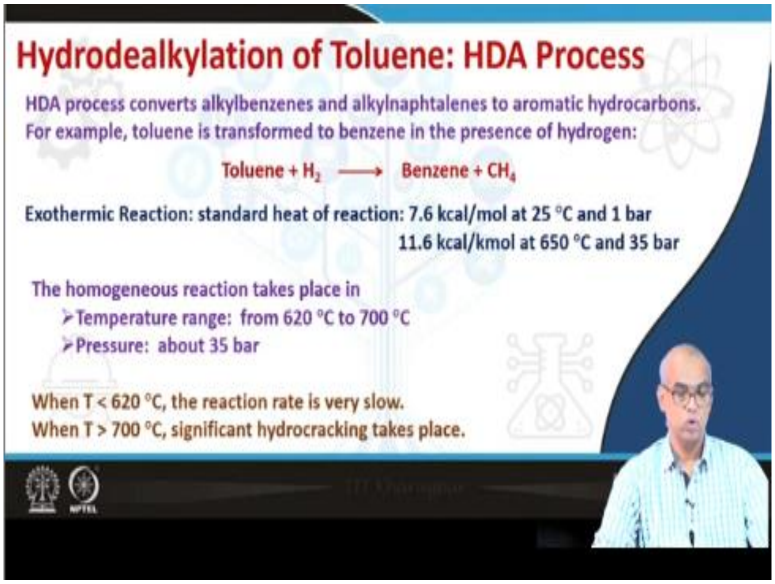

So let us now talk about Hydrodealkylation of Toluene: HDA. HDA process converts alkylbenzenes and alkyl naphthalenes to aromatic hydrocarbons. For example, toluene is transformed to benzene in the presence of hydrogen. So toluene reacts with hydrogen to produce benzene and methane. So we consider toluene, we had hydrogen, this CH3 goes and you get benzene + methane. This is an exothermic reaction. The standard heat of reaction is 7.6. kilocalorie per mole at 25 degree celsius and 1 bar.

And the standard heat of reaction is 11.6 kilocalorie per kilomole at 650 degree Celsius and 35 bar. The homogeneous reaction takes place in the temperature range of 620 degree celsius to 700 degrees celsius and pressure above 35 bar. The temperature range of 620 to 700 is taken because when temperature is less than 620 degrees celsius the reaction rate is very slow. While when temperature goes above 700 degrees celsius, there is significant hydrocracking. So the temperature is chosen from 620 to 700 degree celsius.

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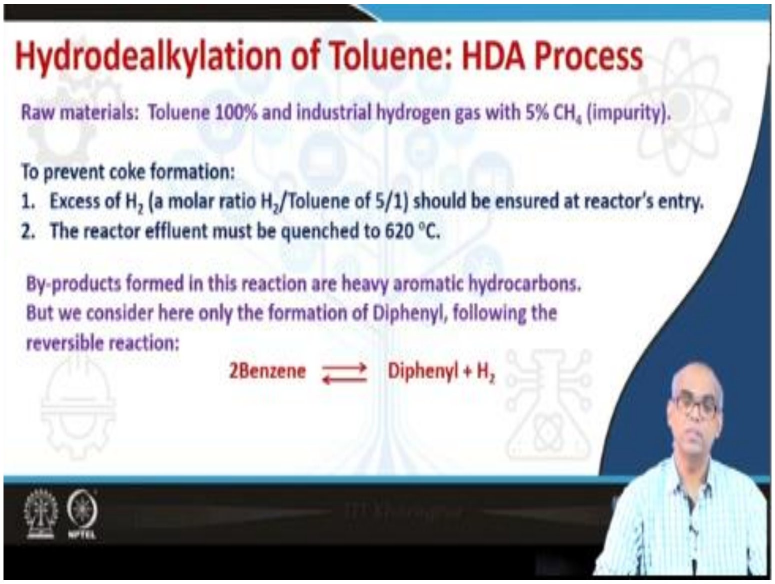

The raw material used is pure toluene, so 100% toluene and industrial hydrogen gas which will contain about 5% of methane as impurity. Industrial hydrogen gas will generally content methane as impurity because almost 50% of Hydrogen is produced by stream reformation of natural gas. So methane comes as impurity. To prevent coke formation during the process, we use excess hydrogen. So molar ratio hydrogen is to toluene of 5 is to 1 should be ensured at reactor's entry.

Also, the reactor effluent must be going to 620 degree celsius. So, these two are done to prevent coke formation. By-products formed in this reaction are heavy aromatic hydrocarbons, but we consider here only the formation of diphenyl and the diphenyl is formed through a reversible reaction where two molecules of benzene reacts reversibly to give you one molecule of diphenyl and one molecule of benzene.

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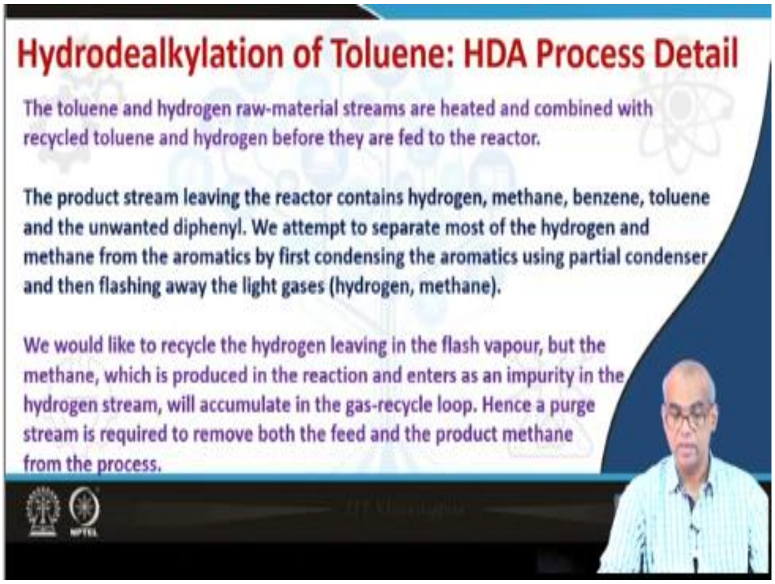

The toluene and hydrogen raw material streams are heated and combined with recycled toluene and hydrogen before they are fed to the reactor. So let us first quickly go through the details of HDA process and then on the basis of this description will try to come up with an intuitive flow sheet for the process. So first the toluene and hydrogen row material streams are heated and combined with recycle toluene and hydrogen before they are fed to the reactor.

The product stream leaving the reactor contains hydrogen, methane, benzene, toluene and the unwanted diphenyl. So there is product as well as unwanted by-product, also the unreacted stuff. We attempt to separate most of the hydrogen and methane from the aromatics by first condensing the aromatics using partial condenser and then flashing away the light gases which are hydrogen and methane. We would like to recycle the hydrogen leaving in the flash vapour.

But the methane which is produced in the reaction and also enters as an impurity in the hydrogen stream will accumulate in the gas recycle loop. Hence a purge stream is required to remove both the feed and the product methane from the process.

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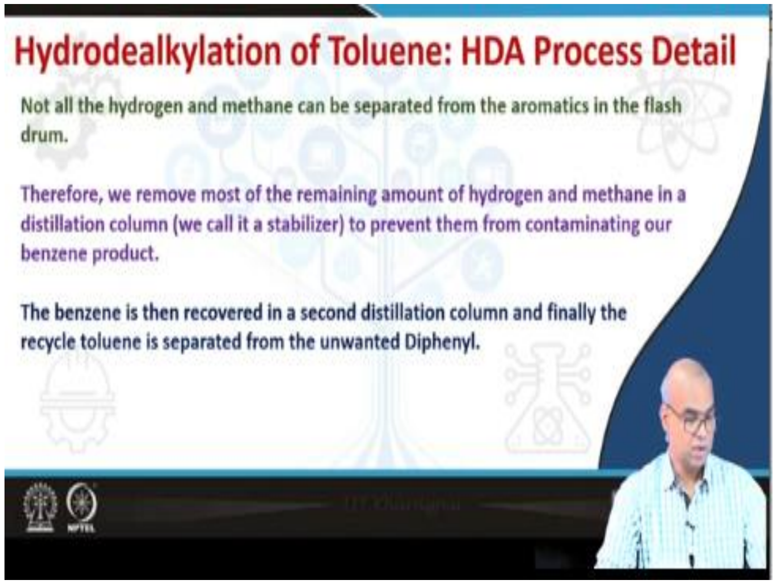

Not all the hydrogen and methane can be separated from the aromatics in the flash drum because it is never a 100% stream. Therefore, we remove most of the remaining amount of hydrogen and methane in a distillation column; we will call it a stabilizer, to prevent them from contaminating our desired product that is benzene. The benzene is then recovered in a second distillation column and finally recycle toluene is separated from the unwanted diphenyl.

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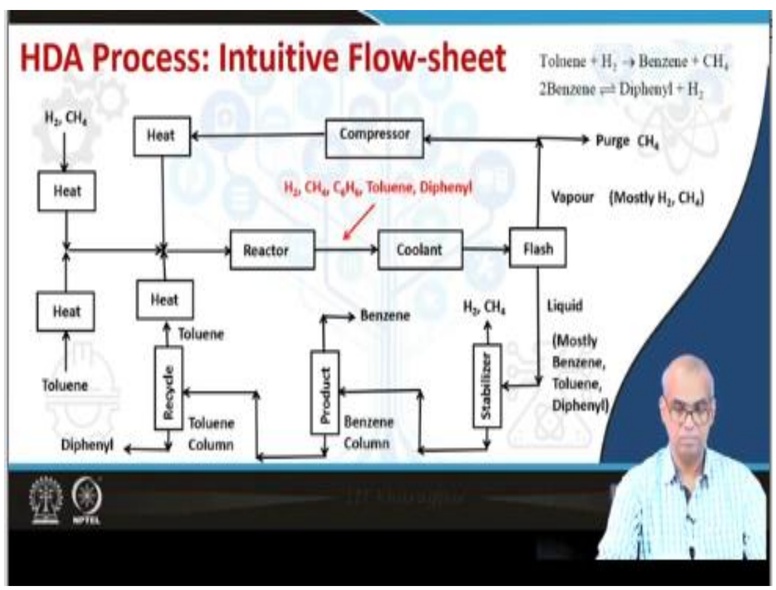

Now on the basis of this, let us develop an intuitive flow sheet. So hydrogen and methane are heated, also toluene which is a liquid under a normal condition is heated to vaporize and also heated to raise the temperature. Then these are mixed and fed to the reactor. So the reactor's stream, the stream that comes out from the reactor, reactor effluence stream will contain the desired product benzene, the undesired by-product diphenyl and also hydrogen methane and toluene.

Now, we will cool this reactor effluence stream and they will go for flash. After flash will have a vapour stream which will mostly contain hydrogen and methane and a liquid stream which will mostly contain benzene, toluene and diphenyl but also we will have some dissolved hydrogen and methane. Now, from the vapour stream, we would like to purge out the methane and the hydrogen will be sent back to the reactor after passing through compression and also before feeding to the reactor the hydrogen stream will be heated up.

Now let us focus your attention on the liquid stream that comes out of the flash drum. As we discussed it mostly contains benzene, toluene and diphenyl, but will also have undissolved light gases hydrogen and methane. So this stream is first sent to a distillation column which we call stabilizer where hydrogen and methane will come out as a top product. The bottom product which will mostly be benzene, toluene and diphenyl will go as feed to the second distillation column which we also call benzene column and benzene will come out as our desired product from top of the distillation column.

The bottom product will contain mostly toluene and diphenyl which will go to the third distillation column which will call toluene column and this mixture will be separated as overhead toluene product which will be heated up and sent back to the reactor as recycle. From the bottom the undesired diphenyl can be taken out. So, this is the intuitive flow sheet that we could develop from the description of the process.

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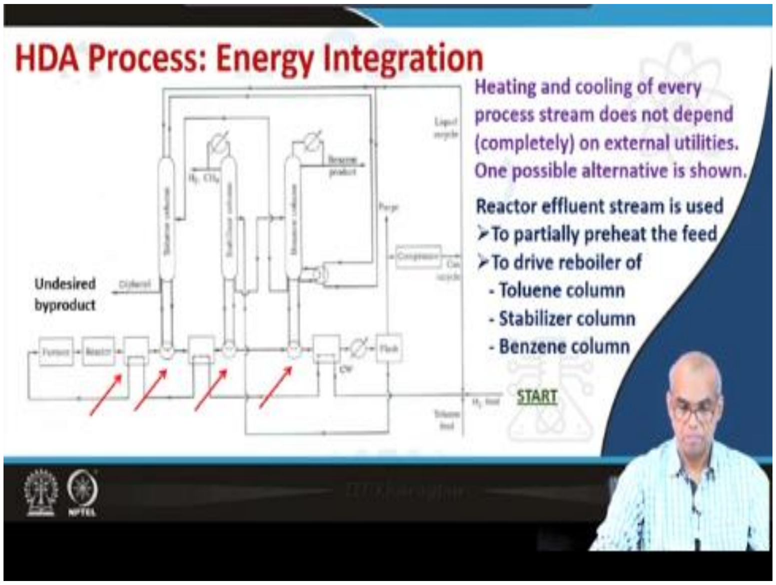

Now, the flow sheet that we just discussed is definitely not an efficient flow sheet because heating and cooling of every process stream depends on external utilities. Now, an efficient flow sheet or efficient process will try to recover waste heat from the process. So it will try to perform energy integration where heating and cooling of every process stream will not depend, at least completely on external utilities. One such possibility is shown on the screen.

Here if you see, the reactor effluent stream is used to partially feed, partially preheat the feed. The reactor effluent stream which is this is also used to drive reboiler of toluene column, the stabilizer column as well as benzene column. So we are doing some amount of heat integration where we are utilizing the energy available with the reactor effluent stream.

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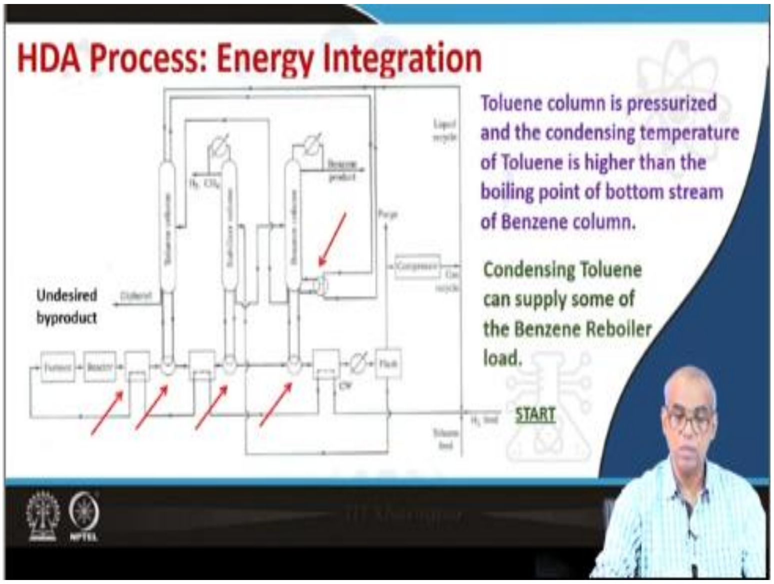

Now the toluene column is pressurized and the condensing temperature of toluene is higher than the boiling point of bottom stream of benzene column. If that is the case, then the condensing toluene can supply some of the benzene reboiler load. So what we just saw is some amount of energy integration in the process.

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But you could also realize that the flow sheet which involves energy integration has many more interconnections and thus is more complicated to analyze. To apply energy integration, we must know flow rate, composition and temperature of every process stream. We should also note details of process heat load. This requires that we fix most part of the flow sheet. Therefore, it is quite natural that we consider the energy integration analysis as the last step in our process design procedure.

So, what we could, conclude that the energy integration should be taken as the last step. Now, we will go on analyzing other steps of the process and we will try to see whether there exists an hierarchy of decisions or not. The decision that we just showcase that energy integration should be taken as a last step. So we will also try to see when should we design the separation process, when should we design the reactor and the recycle etcetera.

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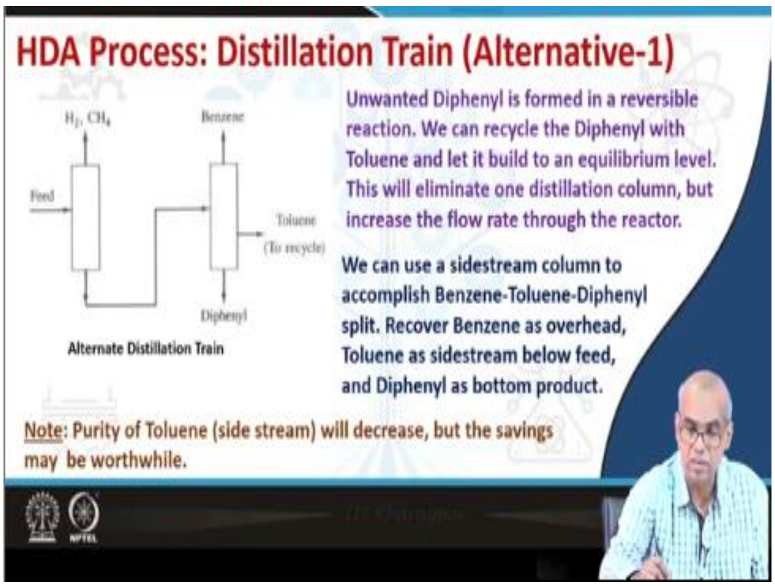

Now, let us focus our attention on the distillation train. Unwanted diphenyl is formed in a reversible reaction. We could recycle the diphenyl with toluene and let it to build to an equilibrium level. This was possible because unwanted diphenyl is formed in a reversible reaction. So this is possible that we can recycle diphenyl with toluene and let it build to an equilibrium level. If we do that, it will eliminate one distillation column, but will increase the flow rate through the reactor.

Look at the sequence of two distillation columns. This is the feed which is basically nothing but a mixture of hydrogen, methane, diphenyl and toluene. Now in the entity flow sheet we have seen that there are sequence of three distillation columns – stabilizer, benzene column and the toluene column. Now, do you require all this 3 distillation columns or can you do with 2 columns? Focus your attention here we can use a side stream column to accomplish benzene diphenyl, toluene split.

We can recover benzene as overhead and toluene as side stream below the feed rate and diphenyl as bottom product. So this is one possible alternative. If we follow this, the purity of toluene of course will decrease because it is not being withdrawn as a top product, but is being withdrawn as a side product. So purity of the toluene will decrease but the savings may be worthwhile and we can actually consider this.

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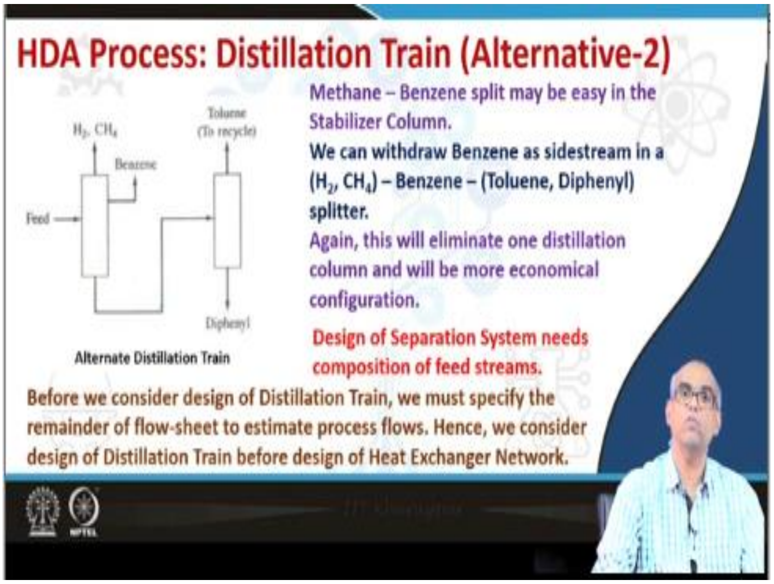

Now there is another alternative. The methane-benzene split may be easy in the first column that is stabilizer column. So you can withdraw benzene as side stream in a hydrogen-methane benzene toluene diphenyl splitter. Again this will eliminate one distillation column and will be more economical configuration. What you see that the design of separation system needs composition of feed streams. So before you consider design of distillation train, we must specify the remainder of the flow sheet to estimate process flows.

Hence, we consider design of distillation train before design of heat exchanger network. So this is the conclusion that we could do after the conclusion that we have made previously that heat integration will be the last step. So now it conclude that design of heat exchanger network will be done at the last, but design of distillation train will be done before the design of heat exchanger network.

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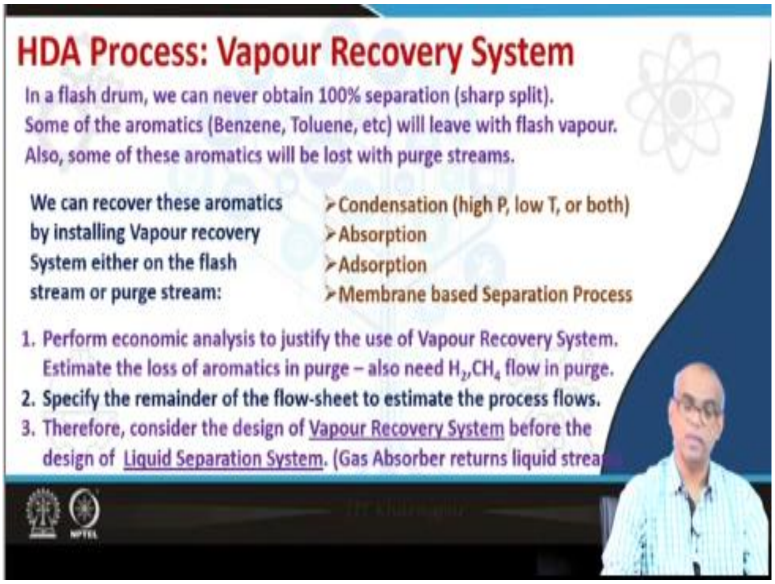

Now vapour recovery system. In a flash drum, we can never obtain 100% separation. Some of the aromatics such as benzene and toluene will leave with flash vapour. Also some of these aromatics will be lost with purge streams. So what we do? We can recover these aromatics by installing vapour recovery system either on the flush stream or purge stream. What can be these vapour recovery systems? Condensation at high temperature or low temperature, at high pressure, at high pressure or low temperature or both.

It may be absorption process, it may be a adsorption process or you can also employ membrane based separation process. Now, we need to perform an economic analysis to justify the use of vapour recovery system. So you have to estimate the loss of aromatics in the purge. So if the loss is considerable, we must go for a vapour recovery system. So we need hydrogen and methane flow in the purge. So these flow rates are required to perform an economic analysis.

So you have to specify the remainder of the flow sheet to estimate the process flows. So therefore, we consider the design of vapour recovery system before the design of liquid separation system. For example, consider we have chosen absorption as vapour recovery system. Now the absorption column will give out a liquid stream which has to go to liquid separation system. So we must design vapour recovery system first before we do the design of liquid separation system. So that is another decision we just make.

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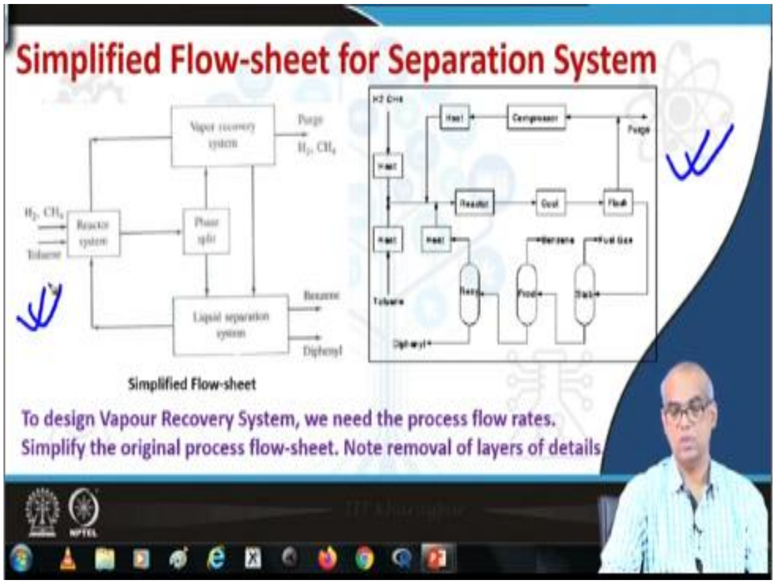

To design vapour recovery system, we need the process flow rates. So you can simplify the original process flow sheet. How? We can club these liquid separation systems which are sequence of distillation columns. So we have lumped this distillation train as a single liquid separation system. Similarly, we also have a vapour recovery system. So we have been able to remove the layers of details from this original flow sheet and obtain this simplified flow sheet which we can use to compute the process flows or process flow rates.

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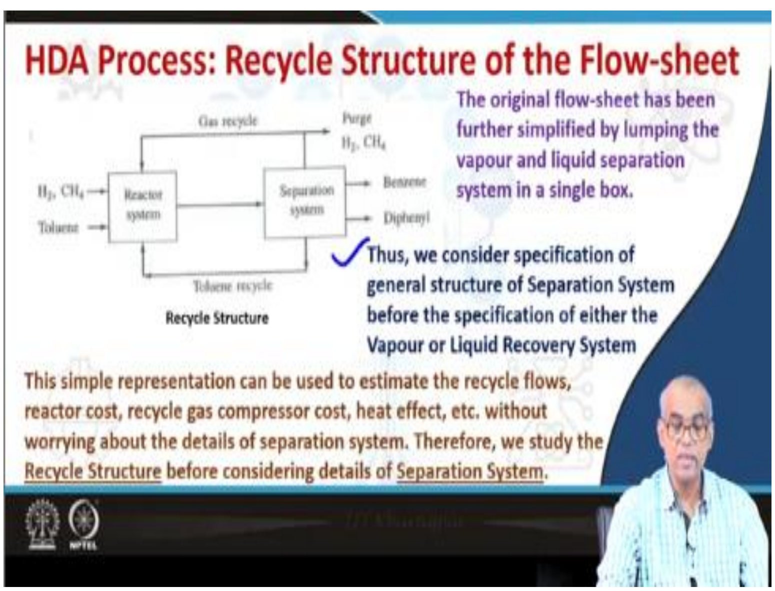

We can further simplify the process flow sheet by lumping the vapour and liquid separation system in a single box. In the previous one, you see we had one box for liquid separation system and another box for vapour recovery systems. Now, we further simplify the flow sheet by lumping the vapour and liquid separation system in a single box. We consider specification of general structure of separation system before the specification of either the vapour or liquid recovery system.

This simple representation can be used to estimate the recycle flows, reactor cost, recycle gas compression cost, heat effects etcetera without worrying about the details of separation system. Therefore, we study the recycle structure before considering details of separation system. So this simple representation of the original process flow sheet can be used to estimate the recycle flows, the reactor cost, recycle gas compression cost, heat effects etcetera without worrying about the details of separation system.

So therefore, it is possible to study the recycle structure before considering details of separation system. So this is another decision that you could make.

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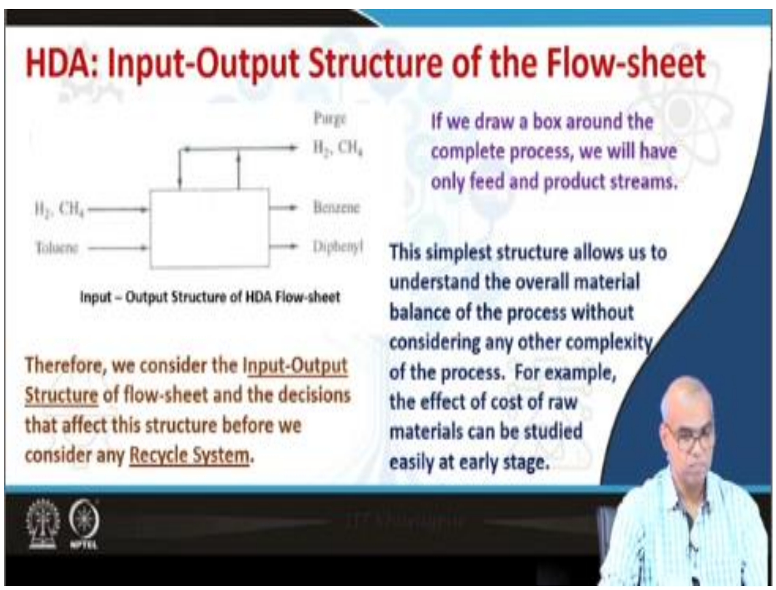

Now, if we draw a box around the entire process, what we will have is, the inputs or the raw material inputs that goes to the process and products and by-products that comes out of the process. So we will only have feed and product streams and this is what you see on the screen now. This simplest structure will allow us to understand the overall material balance of the process without considering any further complexity of the process.

So without considering any further layers of details, we will be able to compute the overall material balance from this simplest input output structure of the flow sheet. For example, the effect of cost of raw materials can be studied easily at such an early stage, with this input output structure of the flow sheet. Therefore, we consider the input output structure of the flow sheet and the decisions that affect the structure before we consider any recycle system.

The consideration of these input output structure of the flow sheet will be enough to write down the overall mass balance. From the mass balance will be able to find out whether the product cost and the reactor cost how do a compare with each other? If the reactor coke, if the reactance cost is more, then there is no point in going further. So, we can consider the input output structure of the flow sheet and the decision that affects the structure before we consider any further details, the next details, immediate details was recycle stream. So before recycle stream, we must consider input output structure.

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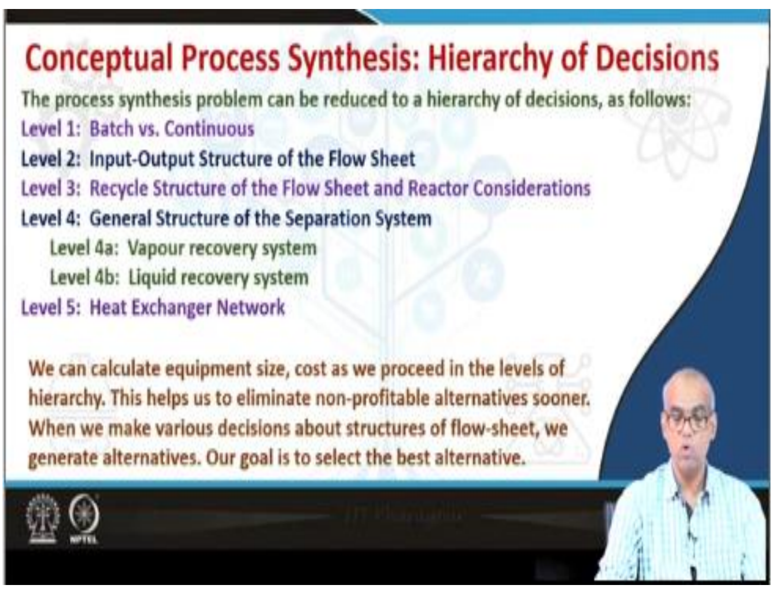

So, what we could see from the discussion of this Hydrodealkylation process of the toluene that there are several layers of decisions. So there is hierarchy of decisions. So the process synthesis problem can be reduced to hierarchy of decision as follows. In the level 1, you can consider whether the process will be a batch or continuous. Level 2 will establish input output structure of the process flow sheet. Level 3, recycle structure of the process flow sheet and reactor considerations.

In the level 4, we will consider general structure of the separation system, first we will talk about vapour recovery system then we will take decision about liquid recovery system. And at the final level that strip level, we can decide on heat exchanger network. So this is the hierarchy of the decisions that can be followed to develop a process flow sheet through hierarchical approach. We can calculate equipment size, cost as we proceed in the levels of hierarchy.

This helps us to eliminate non-profitable alternatives as soon as they appear without going further down in the design process. When we make various decisions about structures of flow sheet, we essentially generate alternatives and our goal is to select the best alternatives.

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Now, we start our discussion on decision at level 1 which is batch versus continuous.

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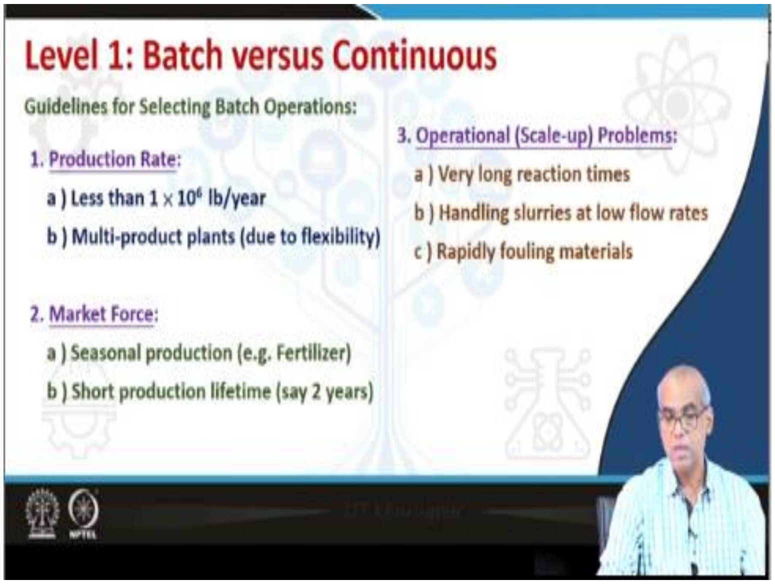

Now, there are certain guidelines for selecting batch operations. So these are the heuristics available which will give you as design guidelines, which will be used as design guidelines to figure out whether we should go for a batch operation or continuous operation. The decisions are based on production rates. If the production rate is less than 1 into 10 to the power 6 pound per year, we go for batch process. Multi product plants due to flexibility will be batch operations.

Market force also determines whether it will be batch or continuous. If the product is a seasonal product, so there will be seasonal production such as fertilizer, we will go for batch operations. If the product has a short lifetime say for two years, it is better to go for batch operation, because a large scale continuous operations, the continuous plant can itself take 3 years to be developed. Operational or scale up problems - very long reaction times, handling slurries is at flow rates low flow rates or rapidly fouling materials will favour batch operations

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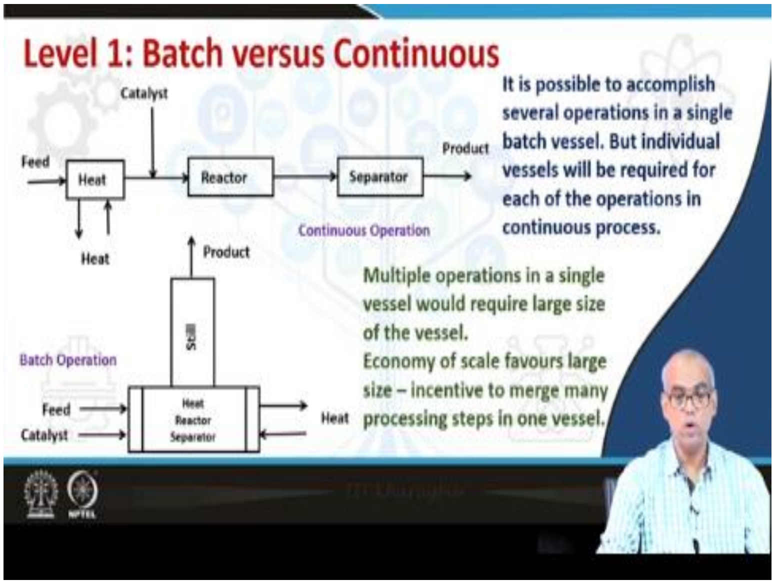

It is possible to accomplish several operations in a batch vessel, but individual vessels will be required for each of the operations in continuous process. Look at the flow sheet for the continuous operation. The equipment that you see, reactors, separators etcetera will be required for individual operations. Whereas for a batch operation the reboiler that you see can be used to supply heat, it can perform the role of reactor, it can also perform the role of separator.

So, multiple operations in a single vessel is possible for batch operation. But multiple operations in a single vessel would require large size of the vessel. Economy of scale favours large size. So there is an incentive to merge many processing states in one vessel. So these are the heuristics or guidelines which can be used to select whether we should go for a batch operation or continuous operation. So we stop our discussions for lecture 27 here and in the next lecture we will talk about the other levels of decisions.