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

## Lecture No -30
## Hierarchical Approach to Process Synthesis - IV

Welcome to lecture 30 of plant design and economics. In this module, we have been talking about conceptual process synthesis and we have particularly paid our attention to hierarchical approach to process synthesis. In the past lectures we have talked about decisions at level 1, level 2 and level 3. In this last lecture of this module, we will talk about decisions at level 4 and level 5 and then we will give a very very brief introduction to algorithmic approach to process synthesis.

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Conceptual Process Synthesis

Today's Topic:

- Hierarchical Approach to Process Synthesis: Decisions at Level-4 and Level-5
- Brief Introduction to Algorithmic Approach to Process Synthesis

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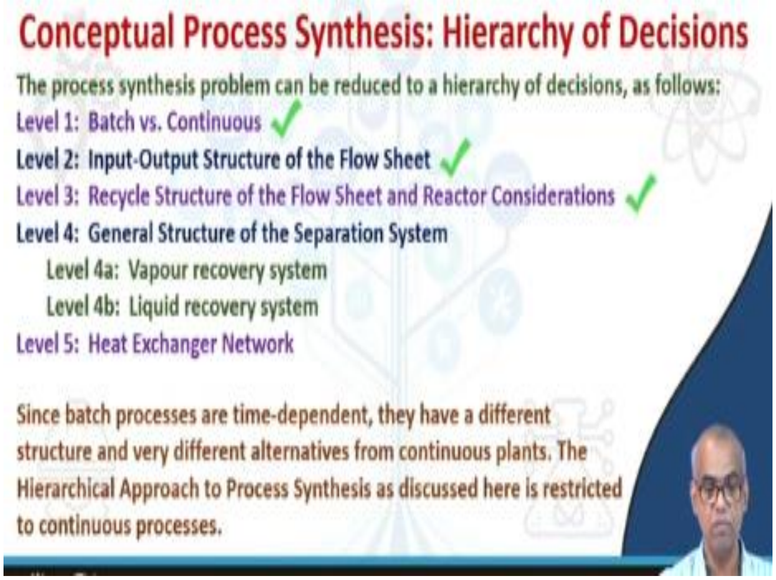

## Conceptual Process Synthesis: Hierarchy of Decisions

The process synthesis problem can be reduced to a hierarchy of decisions, as follows:

Level 1: Batch vs. Continuous ✓
Level 2: Input-Output Structure of the Flow Sheet ✓
Level 3: Recycle Structure of the Flow Sheet and Reactor Considerations ✓
Level 4: General Structure of the Separation System
    Level 4a: Vapour recovery system
    Level 4b: Liquid recovery system
Level 5: Heat Exchanger Network

Since batch processes are time-dependent, they have a different structure and very different alternatives from continuous plants. The Hierarchical Approach to Process Synthesis as discussed here is restricted to continuous processes.

So we have already talked about level 1, level 2 and level 3 decisions. Let us move on to decision level 4 and level 5.

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## Decision At Level 4: Synthesis of Separation System

Decision level 4 is about synthesis of separation system.

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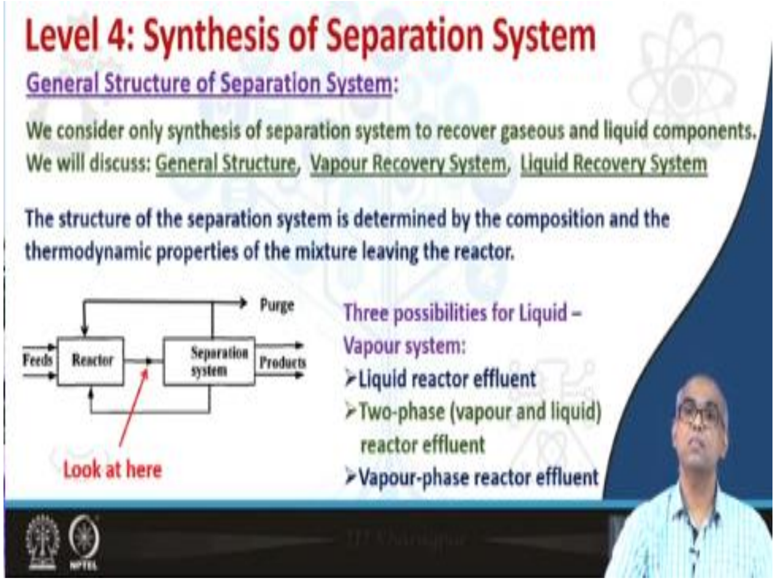

Level 4: Synthesis of Separation System

General Structure of Separation System:

We consider only synthesis of separation system to recover gaseous and liquid components.
We will discuss: General Structure, Vapour Recovery System, Liquid Recovery System

The structure of the separation system is determined by the composition and the thermodynamic properties of the mixture leaving the reactor.

Three possibilities for Liquid – Vapour system:
- Liquid reactor effluent
- Two-phase (vapour and liquid) reactor effluent
- Vapour-phase reactor effluent

Now first we will talk about general structure of the separation systems. Please note that during our discussion on synthesis of separation system we will consider only synthesis of separation systems to recover gaseous and liquid components. So we consider gaseous components and liquid components only and our discussion will be broken into three parts. First we will talk about general structure of the separation system, then we talk about vapour recovery system and then we will talk about liquid recovery system or liquid separation system.

The structure of the separation system will be determined by the composition and the thermodynamic properties of the mixture that comes out from the reactor. So the reactor effluent determines the structure of the separation system. So first task will be to look at the composition and the thermodynamic properties of the reactor reference stream. For liquid vapour systems, we may have 3 distinct possibilities.

The reactor effluent may be a liquid stream, the reactor effluent may be a two phase stream that means a mixture of liquid and vapour or the reactor effluent may be a completely vapour phase stream. So now we will talk about these three cases one by one.

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## Level 4: Synthesis of Separation System

General Structure of Separation System: 1. Liquid Reactor Effluent:

Here, we only need a Liquid Separation System, such as:
- Distillation Columns
- Extraction Units
- Azeotropic Distillation, etc

We normally do not need Gas Absorber, Gas Adsorption unit, etc.

First the general structure of the separation system when your reactor effluent is a liquid stream. Look at the pictorial representation or block diagram representation, the flow sheet. Here we only need a liquid separation system. What kind of liquid separation systems may be distillation columns, extraction units, azeotropic distillation units etcetera based on the particular process at hand.

But we normally do not need gas absorption column or gas adsorption column etcetera; Because we only need liquid separation system.

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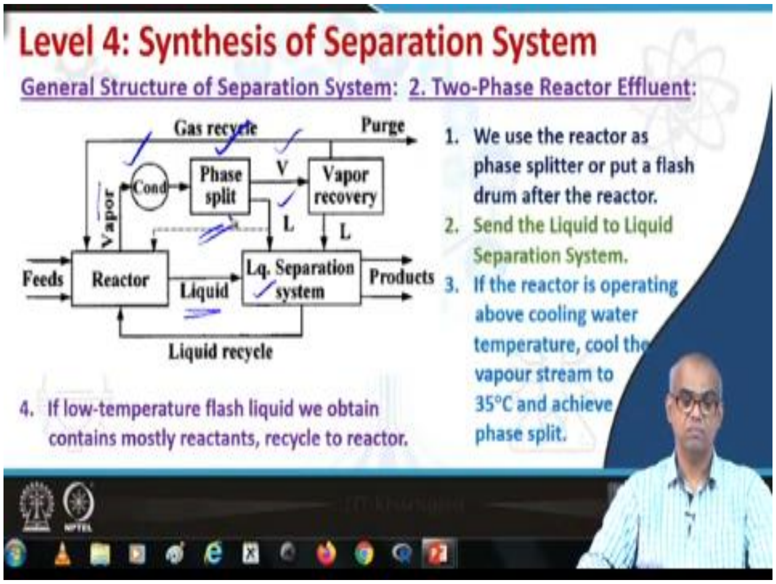

## Level 4: Synthesis of Separation System

General Structure of Separation System: 2. Two-Phase Reactor Effluent:

1. We use the reactor as phase splitter or put a flash drum after the reactor.
2. Send the Liquid to Liquid Separation System.
3. If the reactor is operating above cooling water temperature, cool the vapour stream to 35°C and achieve phase split.
4. If low-temperature flash liquid we obtain contains mostly reactants, recycle to reactor.

Now, let us go to the second possibility where your reactor effluent stream is a two phase mixture. So what will be the general structure of the separation system there? So we use the reactor as phase splitter or we can also put a flash drum after the reactor. So the reactor stream can go to a flash drum or the reactor itself can be used as a splitter. Now, let us consider from the reactor we are getting a liquid stream and a vapour stream.

Now the liquid stream can go to the liquid separation system. So liquid stream goes to liquid separation system. What about the vapour stream? Now if the reactor is operating above cooling water temperature, we will first cool the vapour stream to 35 degrees Celsius and then achieve a phase split. So first cool the vapour stream, we first cool the vapour stream using condenser to 35 degree Celsius and then perform phase split.

So you have a vapour stream and a liquid stream. if the low temperature flash liquid, we obtain contains mostly reactant will recycle the stream to the reactor.

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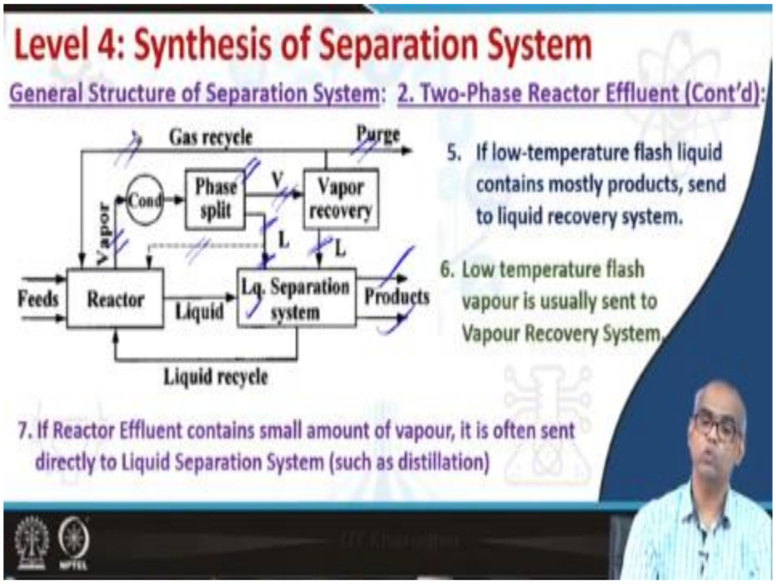

Level 4: Synthesis of Separation System

General Structure of Separation System: 2. Two-Phase Reactor Effluent (Cont'd):

5. If low-temperature flash liquid contains mostly products, send to liquid recovery system.
6. Low temperature flash vapour is usually sent to Vapour Recovery System.
7. If Reactor Effluent contains small amount of vapour, it is often sent directly to Liquid Separation System (such as distillation)

If it mostly contains the products will send it to liquid recovery system. The low temperature flash vapour will be sent to vapour recovery system. Note that from the vapour recovery system a liquid stream may be generated which can be sent to the liquid separation system. However, if the reactor effluent contains only small amount of vapour, then it is often send directly to liquid separation system such as distillation.

So what we learnt is that the reactor itself can be a phase splitter or there may be a phase splitter after the reactor. Now the liquid stream that comes from the reactor can go to liquid separation system and the vapour can be condensed and then vapour can be cooled down to 35 degrees Celsius.

And then phase splitting can occur. After phase splitting you will have a vapour stream and liquid steam, the vapour stream can go to the vapour recovery system and the liquid stream if it mostly contains reactants send it to reactor there is a logical conclusion.

And if it mostly contains products send it to liquid separation system and you will get out the product. Also note that from the vapour recovery systems a liquid stream may be generated which can be sent to the liquid separation system and of course from vapour recovery systems will have a purge stream as well as a gas recycle stream which goes to the reactor. So this will be the general structure for the separation system where you have two phase reactor effluent.

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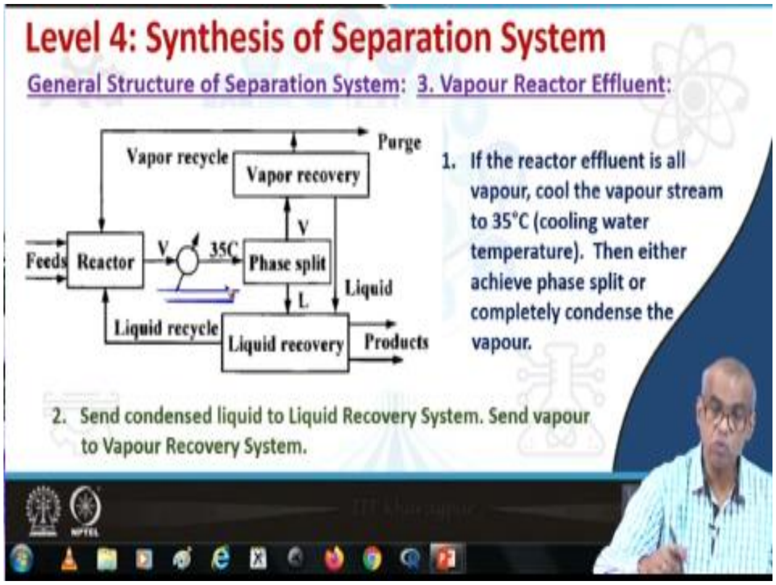

Level 4: Synthesis of Separation System

General Structure of Separation System: 3. Vapour Reactor Effluent:

1. If the reactor effluent is all vapour, cool the vapour stream to 35°C (cooling water temperature). Then either achieve phase split or completely condense the vapour.
2. Send condensed liquid to Liquid Recovery System. Send vapour to Vapour Recovery System.

Now let us consider the third possibility where your reactor effluent is all vapour. If the reactor effluent is all vapour cool the vapour stream to 35 degrees Celsius. 35 degree Celsius is the cooling water temperature then either achieve phase plate or completely condense the vapour. So you have only vapor stream you either phase split and then you get a vapour stream and liquid stream the liquid stem can go to liquid recovery and the vapour stream can go to vapour recovery. Send the condensed liquid to liquid recovery system send the vapour to vapour recovery system.

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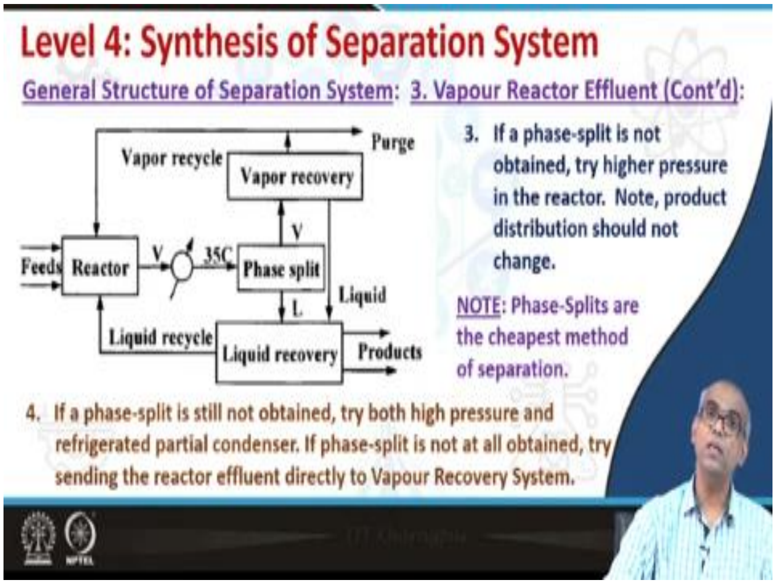

Level 4: Synthesis of Separation System

General Structure of Separation System: 3. Vapour Reactor Effluent (Cont'd):

3. If a phase-split is not obtained, try higher pressure in the reactor. Note, product distribution should not change.

NOTE: Phase-Splits are the cheapest method of separation.

4. If a phase-split is still not obtained, try both high pressure and refrigerated partial condenser. If phase-split is not at all obtained, try sending the reactor effluent directly to Vapour Recovery System.

Now if a phase split is not obtained we need to try higher pressure in the reactor. So let us try a pressurized reactor so that the phase split is possible. However, we must take care that product distribution does not change. If a phase split is still not obtained after using higher pressure, we should try both high pressure as well as refrigerated partial condenser. If phase split is not at all obtained we should try sending the reactor effluent directly to the vapour recovery system.

Now we insist so much on phase splitting because phase splits are the cheapest method of separation. So this will be the general structure of the separation system when you have the reactor effluent as only vapour stream. So reactor effluent is all vapour. So either so cool it down and phase split or condense it.

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## Level 4: Synthesis of Separation System

**Vapour Recovery System:**

**For Synthesis of Vapour Recovery System, We Must Decide:**

1. What type of Vapour Recovery System can be used?
2. What is the best location for the Vapour Recovery System?

**Common Types of Vapour Recovery System:**

- Condensation – high T, low P, both
- Absorption
- Adsorption
- Membrane Separation Process
- Reaction Systems

**Location:**

- The purge stream ✓
- The recycle stream ✓
- The flash-vapour stream ✓

Now let us talk about vapour recovery systems. So we talked about general structure of the separation system. Now, we will talk about vapour recovery systems. After that, we will talk about liquid recovery systems or liquid separation system. Now for synthesis of vapour recovery systems, we have to decide what type of vapour recovery systems can be used and then what is the best location for the vapour recovery systems?

So where are we going to install the vapour recovery systems in your process? These are the two decisions that we have to take now. The common types of vapor recovery systems are condensation at high temperature, low pressure or both. Absorption, adsorption, membrane separation process, reaction systems. So these are common types of vapour recovery systems. So these processes can be used to recover vapour.

Now about location we can put the vapour recovery system on the purge stream, on the recycled stream and also on the flash vapour stream. Now, let us look at the available heuristics which will guide us as to where exactly to put the vapour recovery system.

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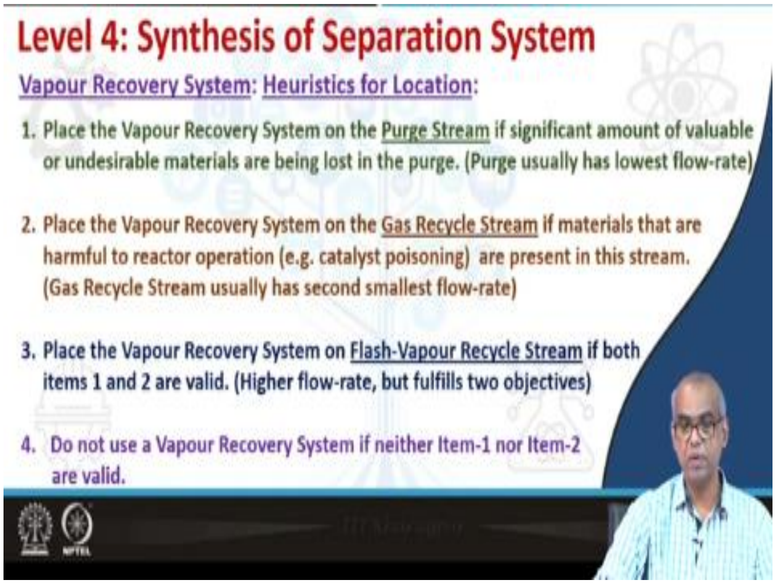

## Level 4: Synthesis of Separation System

Vapour Recovery System: Heuristics for Location:

1. Place the Vapour Recovery System on the Purge Stream if significant amount of valuable or undesirable materials are being lost in the purge. (Purge usually has lowest flow-rate)
2. Place the Vapour Recovery System on the Gas Recycle Stream if materials that are harmful to reactor operation (e.g. catalyst poisoning) are present in this stream. (Gas Recycle Stream usually has second smallest flow-rate)
3. Place the Vapour Recovery System on Flash-Vapour Recycle Stream if both items 1 and 2 are valid. (Higher flow-rate, but fulfills two objectives)
4. Do not use a Vapour Recovery System if neither Item-1 nor Item-2 are valid.

On the purge stream or on the gas recycle stream or on the phase split stream place the vapour recovery system on the purge stream if significant amount of valuable or undesirable materials are being lost in the purge. Note that the purge stream usually has the lowest flow rate. So if significant amount of valuable or undesirable materials are being lost in the purge stream, let us put the vapour recovery system on the purge stream.

Place the vapour recovery system on the gas recycle stream. If materials that are harmful to reactor operation are present in this stream. What kind of harmful components that may be present the gas recycle stream? Say something which will poison in the catalyst. So you would not allow that component to enter the reactor. So we will put the gas recovery system or vapour recovery systems on the gas recycle stream.

Note that gas recycle stream usually has the second smallest flow rate. We place the vapour recovery stream on the flash vapour recycle stream, if both items 1 and 2 are valid, that means you have significant amount of valuable or undesirable materials being lost in the purge stream, as well as you may have harmful components for the reactor on the gas recycle stream. In that case, arrest these components before they go to purge stream or they go to gas recycles stream.

That means we will put it on the flash vapor recycle stream. So do not use a vapour recovery system if neither item 1 or item 2 are valid. That means if you do not have a significant amount of available or undesirable materials being lost neither, you have a harmful component in the gas recycle stream, we do not have to use vapor recovery system.

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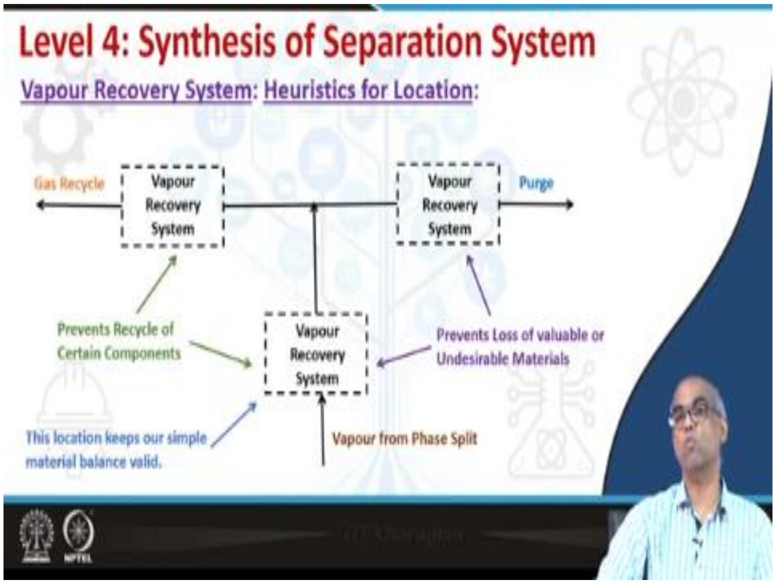

Level 4: Synthesis of Separation System

Vapour Recovery System: Heuristics for Location:

Gas Recycle

Vapour Recovery System

Vapour Recovery System

Purge

Prevents Recycle of Certain Components

Vapour Recovery System

Prevents Loss of valuable or Undesirable Materials

This location keeps our simple material balance valid.

Vapour from Phase Split

So this is schematically shown here. So, this is the vapour stream that comes after phase split. This is the purge stream. So if you put here it will prevent loss of valuable or undesirable material. If you put here it will prevent recycle of say harmful components to the reactors and if you put here it will perform both the objectives. Note that, if we put the vapour recovery systems on the vapour stream that comes after phase splitting, this particular location will keep our simple material balance valid.

Because in our simple material balance we assume 100% recovery. So this can be achieved by putting the vapour recovery systems on the vapour stream coming from the phase split.

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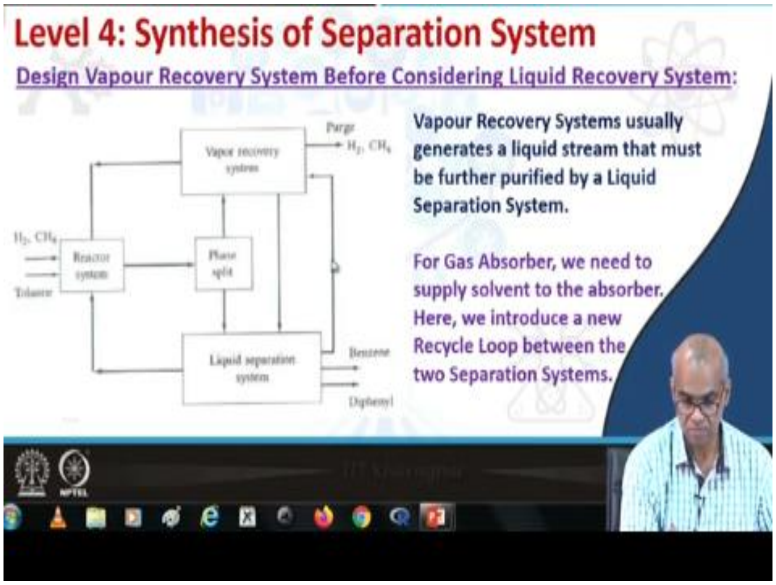

Level 4: Synthesis of Separation System

Design Vapour Recovery System Before Considering Liquid Recovery System:

Vapour Recovery Systems usually generates a liquid stream that must be further purified by a Liquid Separation System.

For Gas Absorber, we need to supply solvent to the absorber. Here, we introduce a new Recycle Loop between the two Separation Systems.

So again you see the schematic for the vapour recovery systems and liquid recovery systems for the HDR process. Now, we consider the design of vapour recovery system before considering liquid recovery system. Vapour recovery systems usually generates a liquid stream that must be further purified by a liquid separation system. For example gas absorption, if you are using gas absorption column for vapour recovery system, it will generate a liquid stream and that you have to send to the liquid recovery system.

So you first consider vapour recovery system next we consider liquid separation system. For gas absorber, we need to supply solvent to the absorber. So here we introduce a new recycle stream between the liquid separation system and vapor recovery system.

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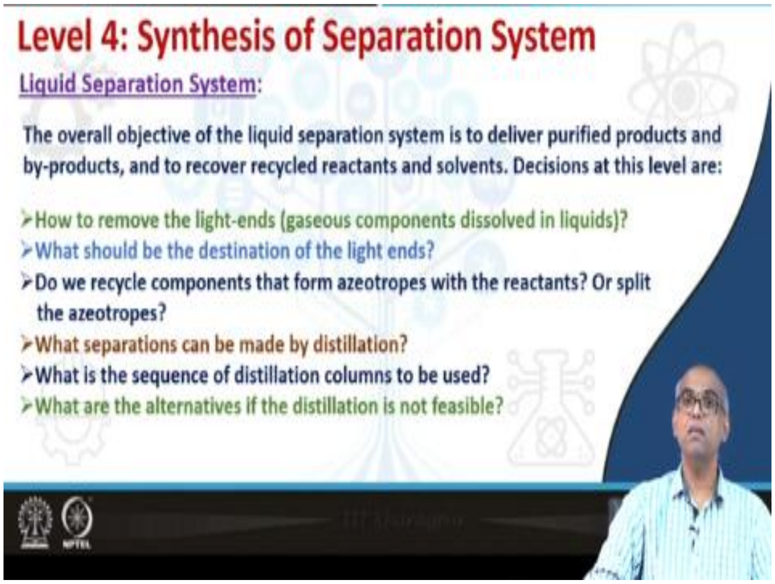

## Level 4: Synthesis of Separation System

Liquid Separation System:

The overall objective of the liquid separation system is to deliver purified products and by-products, and to recover recycled reactants and solvents. Decisions at this level are:

- How to remove the light-ends (gaseous components dissolved in liquids)?
- What should be the destination of the light ends?
- Do we recycle components that form azeotropes with the reactants? Or split the azeotropes?
- What separations can be made by distillation?
- What is the sequence of distillation columns to be used?
- What are the alternatives if the distillation is not feasible?

Now after talking about vapour recovery systems now we can talk about liquid separation system. The overall objective of the liquid separation system is to deliver purified products and by products and to recover recycled reactants and solvents. So what are the decisions at this level? The decisions are how to remove the high ends, how to remove the light ends that is gaseous components that are dissolved in liquids.

What should be the destination of the light ends? Do you recycle components that form Azeotropes with the reactants? Or split the Azeotropes? What separations can be made by distillation? What is the sequence of distillation columns to be used? What are the alternatives if the distillation is not feasible? So those are these are the decisions that you have to take to fix the liquid separation system.

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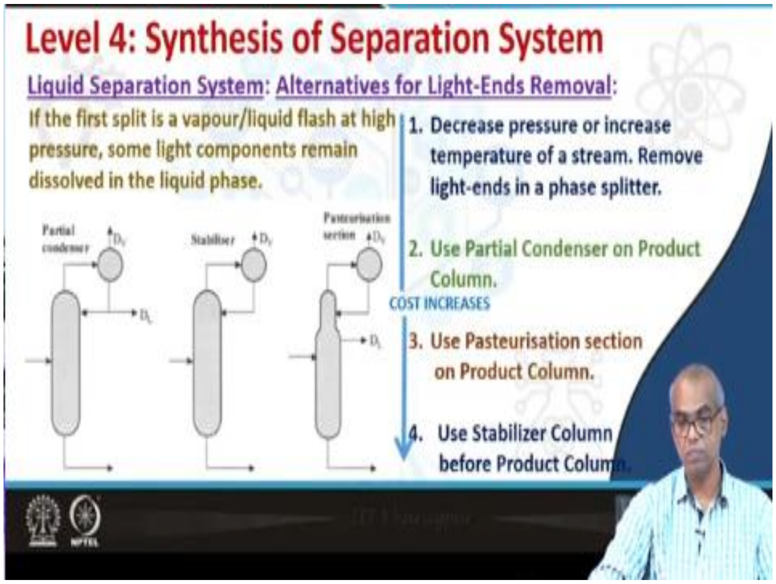

## Level 4: Synthesis of Separation System

**Liquid Separation System: Alternatives for Light-Ends Removal:**

If the first split is a vapour/liquid flash at high pressure, some light components remain dissolved in the liquid phase.

1. Decrease pressure or increase temperature of a stream. Remove light-ends in a phase splitter.
2. Use Partial Condenser on Product Column.
3. Use Pasteurisation section on Product Column.
4. Use Stabilizer Column before Product Column.

COST INCREASES

So, what are the alternatives for light ends removal? So how to separate the light ends? If the first split is a vapour liquid flash at high pressure some light components will remain dissolved in the liquid phase, so these light components must be removed. So, what are the alternatives that we have? We can decrease pressure or increase temperature of a stream remove light ends in a phase splitter.

We can use partial condenser on product column. We can use pasteurization section on product column. We can also use stabilizer column before product column. This is what we have seen in case of HDF process. Remember the stabilizer column was the first distillation column then there was product column benzene column and then finally it was toluene column. Now these are the schematics for partial condenser, for partial condenser both the vapour and the liquid steam comes out from the top of the distillation column.

In case of stabilizer only we take out the vapor stream in case of pasteurization section, we take out the vapour stream and the liquid stream is taken out at the top of the distillation column but not from here, but towards the top of the crystallization column above the feed tray. Now the cost of these options increases as we move from phase splitting to partial condenser to pasteurization section to stabilizer column.

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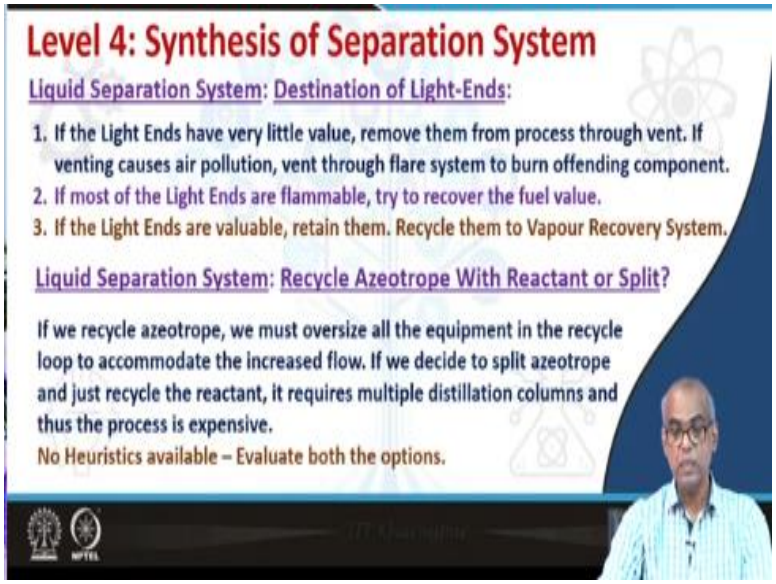

## Level 4: Synthesis of Separation System

**Liquid Separation System: Destination of Light-Ends:**

1. If the Light Ends have very little value, remove them from process through vent. If venting causes air pollution, vent through flare system to burn offending component.
2. If most of the Light Ends are flammable, try to recover the fuel value.
3. If the Light Ends are valuable, retain them. Recycle them to Vapour Recovery System.

**Liquid Separation System: Recycle Azeotrope With Reactant or Split?**

If we recycle azeotrope, we must oversize all the equipment in the recycle loop to accommodate the increased flow. If we decide to split azeotrope and just recycle the reactant, it requires multiple distillation columns and thus the process is expensive.

No Heuristics available – Evaluate both the options.

So what are now, the destination of the light ends? What do you do with this light components? If the light ends have very little value remove them from the process through vent. Now, you may have offending components and you may not be allowed to vent it directly to the atmosphere because they may cause air pollution. Then will vent this components through flare system and in the flare system will burn the offending components.

If most of the light ends are flammable, we try to recover the fuel value. If the light ends are valuable components, we would like to retain them in the process. So we will recycle them to the vapour recovery system. So this will be our destination for light ends. Next decision, we have to take is about whether to recycle Azeotrope with the reactant or split the Azeotrope and recycle only the reactant.

So if you recycle Azeotrope along with the reactant we must oversize all equipment in the recycle loop to accommodate the increase flow. Note that, during liquid separation there may be formation of Azeotropes. Now, we have to take a decision whether you will recycle this Azeotrope that has been formed along with the reactant or you will split the Azeotrope and take out the reactant and recycle only the reactant.

So if we recycle Azeotrope along with reactant, we must oversize all the equipment in the recycle loop to accommodate the increased flow it will of course invite additional cost. If we decide to split Azeotrope and just recycle the reactant, it requires multiple distillation columns and thus the processes will be expensive.

Now no heuristic is available here and we have to evaluate both the options, we must perform economic evaluations for both the options and take the appropriate decisions, take the cost effective option.

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Level 4: Synthesis of Separation System

Liquid Separation System: Available Separation Processes:

Distillation is the most commonly applied and reliable technique for the separation of liquid mixtures. When distillation is feasible, it should be immediately adopted.

Heuristic-1:

If Relative Volatility > 1.5, the simple distillation is the most economical separation.

For Relative Volatility < 1.1 distillation is not feasible.

For 1.1 < Relative Volatility < 1.5 the column requires very large number of stages and/or very high reflux. Other separation methods could be more appropriate.

Heuristic 2:

The relative volatility may be improved by selecting an appropriate operating pressure. Low pressures enhance the relative volatility, but increases the energy consumption.

What are the available separation processes for liquid separation? Distillation is the most commonly applied and reliable technique for the separation of liquid mixtures. When distillation is feasible, it should be immediately adopted. Now we will talk about 2 heuristics about distillation process. If relative volatility is greater than 1.5 the simple distillation is the most economical separation.

However, you relative volatility is less than 1.1 distillation is not feasible. For relative volatility between 1.1 and 1.5 the column will require very large number of stages and may also require very high reflux. So under such situations other separation methods may be more appropriate so you have to evaluate that option. Heuristic 2 the relative volatility may be improved by selecting an appropriate operating pressure. Low pressure enhance the relative volatility but increases the energy consumption.

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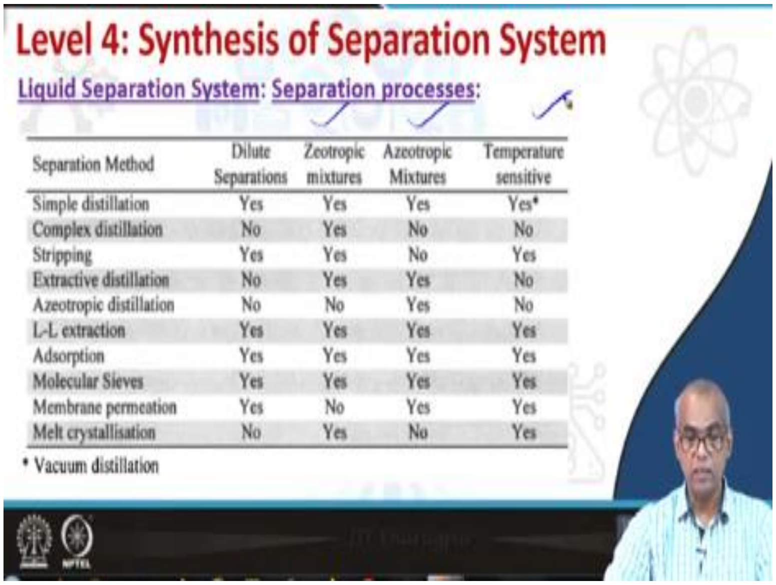

## Level 4: Synthesis of Separation System

**Liquid Separation System: Separation processes:**

| Separation Method | Dilute Separations | Zeotropic mixtures | Azeotropic Mixtures | Temperature sensitive |
|---|---|---|---|---|
| Simple distillation | Yes | Yes | Yes | Yes* |
| Complex distillation | No | Yes | No | No |
| Stripping | Yes | Yes | No | Yes |
| Extractive distillation | No | Yes | Yes | No |
| Azeotropic distillation | No | No | Yes | No |
| L-L extraction | Yes | Yes | Yes | Yes |
| Adsorption | Yes | Yes | Yes | Yes |
| Molecular Sieves | Yes | Yes | Yes | Yes |
| Membrane permeation | Yes | No | Yes | Yes |
| Melt crystallisation | No | Yes | No | Yes |

* Vacuum distillation

Now here we have listed the various separation processes for liquid separation systems; simple distillation, complex distillation, stripping, extractive distillation, Azeotropic distillation, liquid liquid extraction, adsorption, molecular sieves, membrane permeation, melt crystallization etcetera. So whether they are applicable for Azeotropic mixture or geotropic mixtures that means non-azeotropic mixtures or whether they are temperature sensitive all are given. So you can look at this table and can decide about the separation processes.

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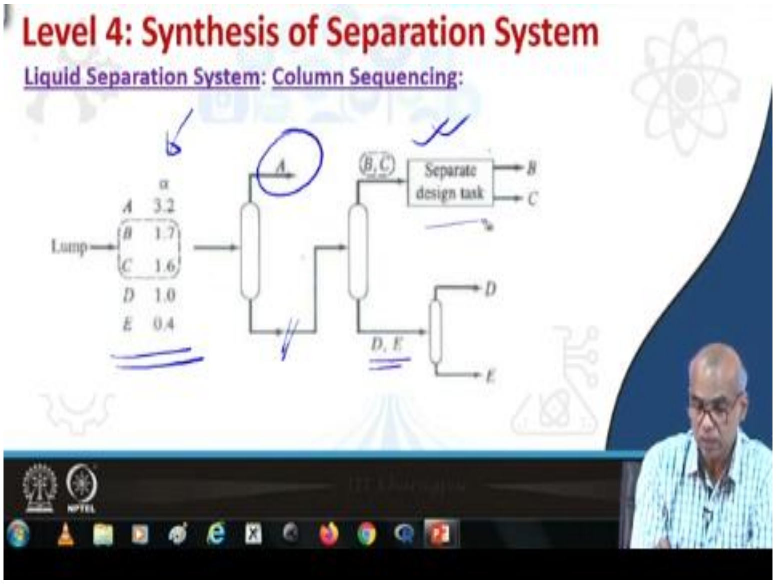

## Level 4: Synthesis of Separation System

**Liquid Separation System: Column Sequencing:**

Now in case of liquid separations using distillation column column sequences is an important decision to take. Think about a mixture with 5 components A, B, C, D, E we are arrange them according to the relative volatility value about in the decreasing order of relative volatility, A has the highest relative volatility B and C have very close relative volatility. Now in the first distillation column the A can be taken out as the top product as more volatile component.

So the bottom product will contain mostly mixture of B, C, D and E, in the second distillation column where it goes as B since B and C are close boiling, B and C can come out as the top product whereas D and E which has differences in relative volatility will come as bottom product which can be further separated into D and E but B and C are very close boiling and distillation may not be appropriate process to separate them. So we design a separate process for separating B and C.

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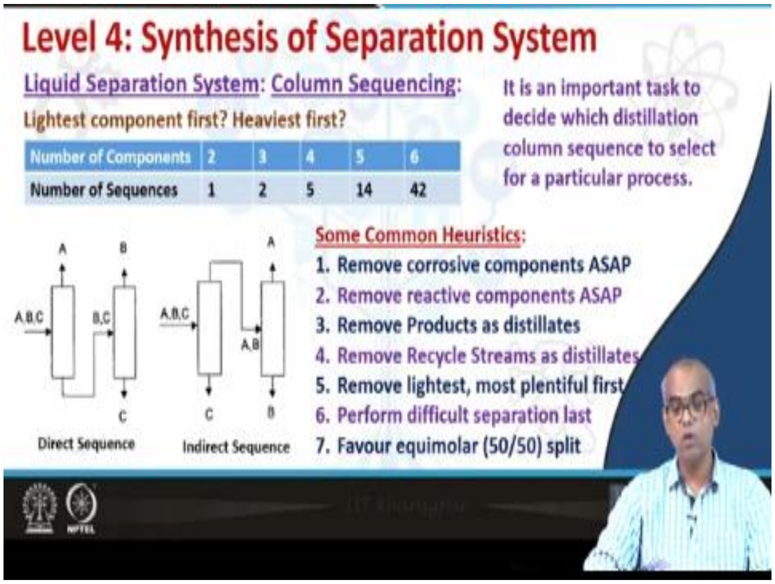

Level 4: Synthesis of Separation System

Liquid Separation System: Column Sequencing:

Lightest component first? Heaviest first?

| Number of Components | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|
| Number of Sequences | 1 | 2 | 5 | 14 | 42 |

It is an important task to decide which distillation column sequence to select for a particular process.

Some Common Heuristics:

1. Remove corrosive components ASAP
2. Remove reactive components ASAP
3. Remove Products as distillates
4. Remove Recycle Streams as distillates
5. Remove lightest, most plentiful first
6. Perform difficult separation last
7. Favour equimolar (50/50) split

So column sequencing is an important task to decide which distillation column sequence to select for a particular process. So we can take out light component first we can also take out heaviest component first. The number of sequences will increase with increasing number of components. If we have 3 components say A, B and C you have 2 possible ways of sequencing the distillation column.

Here in the direct sequence, we take out the lightest component A first and then B and C are separated in the second distillation column. In the indirect sequence as a second option, we can take out the heaviest component C first and then in the second distillation column take out A and

B. Now the problem becomes more and more complex as the number of count of components increase.

You can see that with 6 components, there may be 42 number of sequences. We will talk about this distillation column sequencing more when you talk about synthesis of separation systems in more details in later modules. Here we talk about some common heuristics. Remove corrosive components as soon as possible. Remove reactive components as soon as possible. Remove products as distillates.

Remove recycled streams as distillates. Remove lightest component first. Remove most plentiful component first. Perform difficult separations last and always favour equimolar 50-50 moles split.

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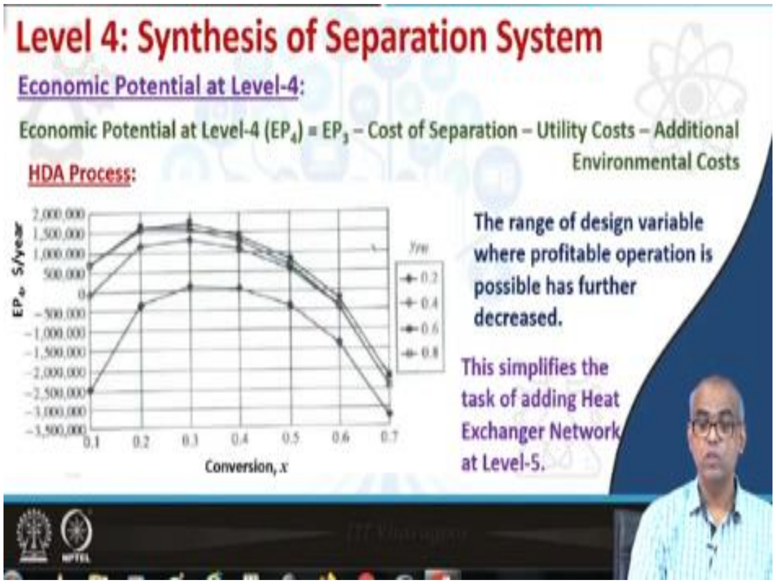

Level 4: Synthesis of Separation System

Economic Potential at Level-4:

Economic Potential at Level-4 ($EP_4$) = $EP_3$ – Cost of Separation – Utility Costs – Additional Environmental Costs

HDA Process:

The range of design variable where profitable operation is possible has further decreased.

This simplifies the task of adding Heat Exchanger Network at Level-5.

Finally, let us talk about economic potential at level 4. So economic potential at level 4, EP4 will be EP3 that is economic potential at level 3 - cost of separation - utility cost - additional environmental cost. Now in the figure we have drawn EP4 economic potential at level 4 versus conversion for various values or hydrogen composition in the purge stream. Note that, it is the design variable, conversion is another design variable.

Now note that the shape of the curve is retained if we consider. Because if you consider EP3 versus conversion and EP4 versus conversion, we see that both as the same general shape where the economic potential source a maximum, but if you compare these two economic potential versus conversion curve for certain given values, these are plotted for certain given values of various cost data.

So that we have been able to put this numbers on the economic potential axis, which is a vertical axis here, so if you do that, we can see that range of design variables where profitable operation is possible has decreased further. So this simplifies the tasks of adding heat exchanger network at the next level, which is level 5.

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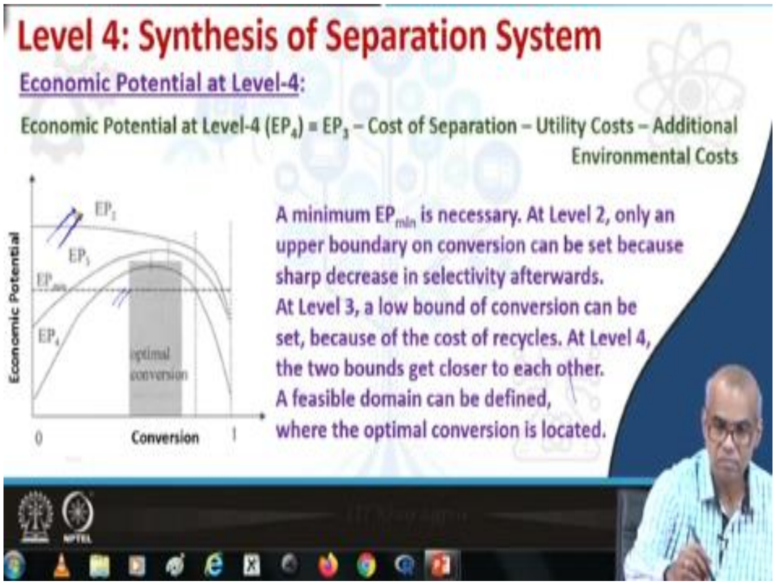

## Level 4: Synthesis of Separation System

Economic Potential at Level-4:

Economic Potential at Level-4 ($EP_4$) = $EP_3$ – Cost of Separation – Utility Costs – Additional Environmental Costs

A minimum $EP_{min}$ is necessary. At Level 2, only an upper boundary on conversion can be set because sharp decrease in selectivity afterwards.
At Level 3, a low bound of conversion can be set, because of the cost of recycles. At Level 4, the two bounds get closer to each other.
A feasible domain can be defined, where the optimal conversion is located.

So this will be more clear if we now plot all EP2, EP 3, EP4 has you see now economic potential versus conversion. Now this horizontal broken line represents a minimum amount of economic potential that must be made otherwise there is no point in going further in the design process. At level 2, we are not able to put any lower bound on the conversion will all only be only available to put a higher bound on the conversion if you remember which was around 0.8.

At level 3, a low bound on the conversion was set because of the cost of the recycles now there was a state of between material cost and recycle costs. At level 4 again we have cost of separation needs to be subtracted from EP3. So at level 4, the lower bounds and upper bounds got closer to each other. Which it means that you are now able to narrow a feasible domain over which the optimal conversion is located.

So the bounds between the lower bound and upper bit bound between the design variables got narrowed down as we go on evaluating economic potential from level 2, level 3 to level 4, so this essentially lowers down my search space for the heat integration work that we perform in the next level. So this is how we can systematically bring down the surface or the feasible domain for the design space.

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Decision At Level 5: Heat Exchanger Network

Now we briefly talk about decision at level 5 heat exchanger network.

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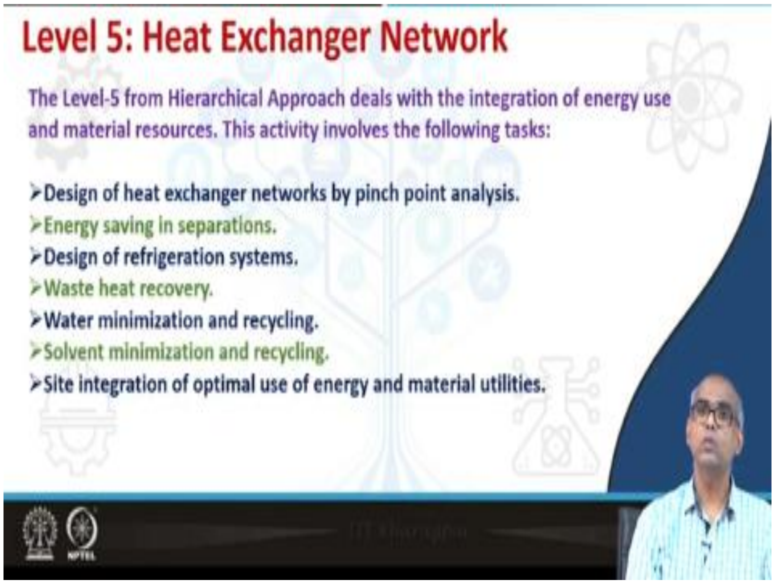

Level 5: Heat Exchanger Network

The Level-5 from Hierarchical Approach deals with the integration of energy use and material resources. This activity involves the following tasks:

- Design of heat exchanger networks by pinch point analysis.
- Energy saving in separations.
- Design of refrigeration systems.
- Waste heat recovery.
- Water minimization and recycling.
- Solvent minimization and recycling.
- Site integration of optimal use of energy and material utilities.

We will talk about this in more details in the later module. The level 5 from hierarchical approach deals with the integration of energy use and material resources. This activity involves the following task. Design of heat exchanger network by pinch point analysis, energy saving in separations, design of refrigeration systems, waste heat recovery, water minimization and recycling, solvent minimization and recycling, site integration of optimal use of energy and material utilities.

So we have now completed all the decisions at level 1 to level 5. If we follow this systematically will be able to come up with a optimal or very close to optimal flow sheet for our process.

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Algorithmic Approach to Process Synthesis

So this was all about the hierarchical approach to process synthesis. Now will briefly in fact very briefly outline the algorithmic approach to process synthesis.

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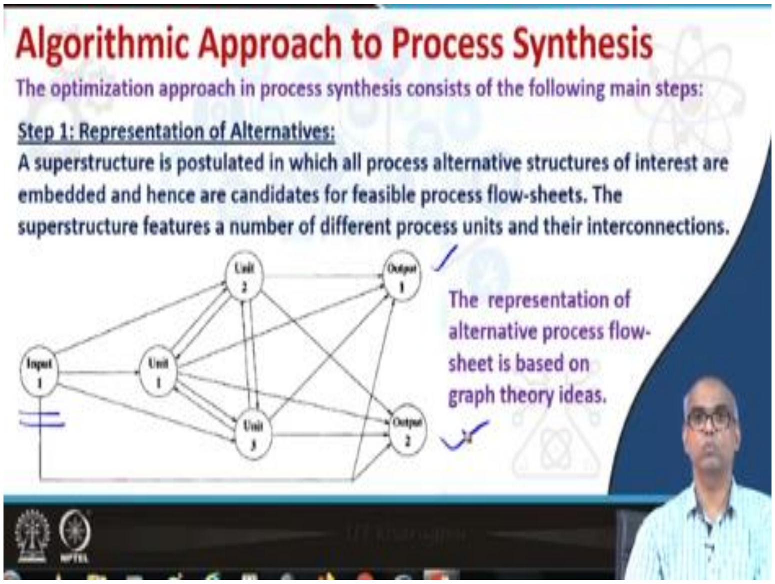

Algorithmic Approach to Process Synthesis

The optimization approach in process synthesis consists of the following main steps:

Step 1: Representation of Alternatives:

A superstructure is postulated in which all process alternative structures of interest are embedded and hence are candidates for feasible process flow-sheets. The superstructure features a number of different process units and their interconnections.

The representation of alternative process flow-sheet is based on graph theory ideas.

The algorithmic approach or the optimization approach in process synthesis consist of the following 3 main steps. Step 1 representation of alternatives. So here also similar here also will have representation of alternatives then we have a mechanism to evaluate the alternatives and we should have a mechanism to find out the base optimal flowship. So in the representation of alternatives a superstructure is postulated in which all possible alternative structures of interest are embedded.

And hence are candidate for feasible process flow sheets. So you have to first generate a superstructure, which is nothing but a collection of all possible or feasible process flow sheets. So one or more very good or optimal flow sheets will be out of these feasible flow sheets. So superstructure will consist of all feasible process flow sheets, the superstructure features a number of different process units and they are interconnections.

So how do you represent this process alternatives. The representation of alternative processes is based on ideas from graph theory. Now look at this schematic look at this diagram you have 3 units. Unit 1, unit 2 and unit 3. One input and 2 output, now all possible interconnections are shown. So this consists this represents a very simple superstructure of a process involving 1 unit, 2 outputs and 1 input, 3 units and 2 outputs, so which is represented by simple graphs.

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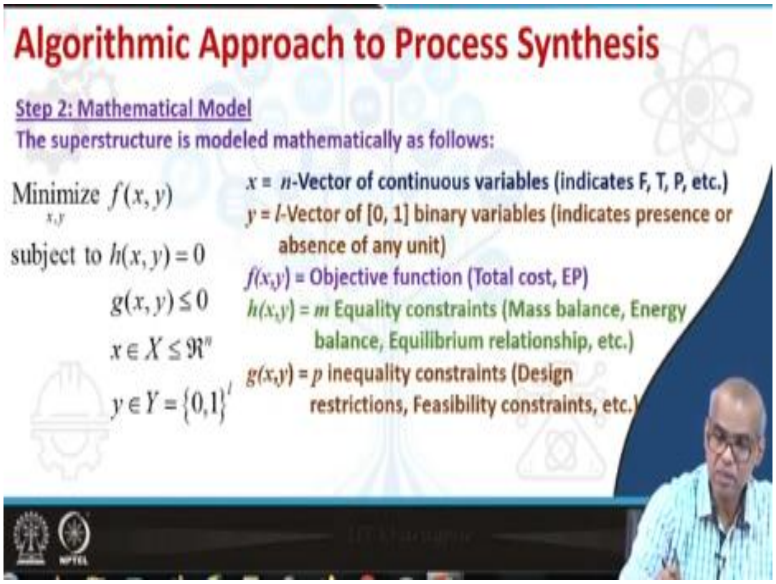

Algorithmic Approach to Process Synthesis

Step 2: Mathematical Model

The superstructure is modeled mathematically as follows:

$$\begin{aligned} &\underset{x,y}{\text{Minimize}}\ f(x,y) \\ &\text{subject to } h(x,y)=0 \\ &\qquad g(x,y)\le 0 \\ &\qquad x\in X\le \Re^{n} \\ &\qquad y\in Y=\{0,1\}^{l} \end{aligned}$$

$x$ = $n$-Vector of continuous variables (indicates F, T, P, etc.)

$y$ = $l$-Vector of [0, 1] binary variables (indicates presence or absence of any unit)

$f(x,y)$ = Objective function (Total cost, EP)

$h(x,y)$ = $m$ Equality constraints (Mass balance, Energy balance, Equilibrium relationship, etc.)

$g(x,y)$ = $p$ inequality constraints (Design restrictions, Feasibility constraints, etc.)

Now in the second stage, which is about mathematical modeling of superstructure, the superstructure is modeled as an optimization problem in particular a mixed integer linear or non-linear programming problem. So you have an objective function to minimize. For example, we want to find out the minimum cost optimal process flow sheet subject to certain constants. Now this objective function f x, y say may represent the total cost or economic potential we want to maximize.

Note that minimization of a function is same as maximization of minus of that function. Now, these are subject to certain constants equality constants which may represent say mass balance, energy balance, equilibrium relationship, etcetera. Inequality constraints which represents the design restriction feasibility constants, etcetera and the objective function is the function of design variables x and y both x and y may be r vectors.

So x is a vector of real numbers. So x is n vector of continuous variables. So it can take on continuous values real values, whereas y takes on only binary variable 0 and 1. So x represents design variables, such as flow rates, temperatures, spacers, etcetera. Whereas y which takes only binary variables will indicate say whether a particular process unit will exist in a flow sheet or not exist.

So 1 means it will exist 0 means you do not exist. So this way, we have formulated a mathematical optimization problem. Note that if this objective function and the constants are nonlinear will have a mixed integer nonlinear programming problem. Why mixed integer? Because some design variables will take on real values some design variables will take on integer values 1 and 0 or binary variables.

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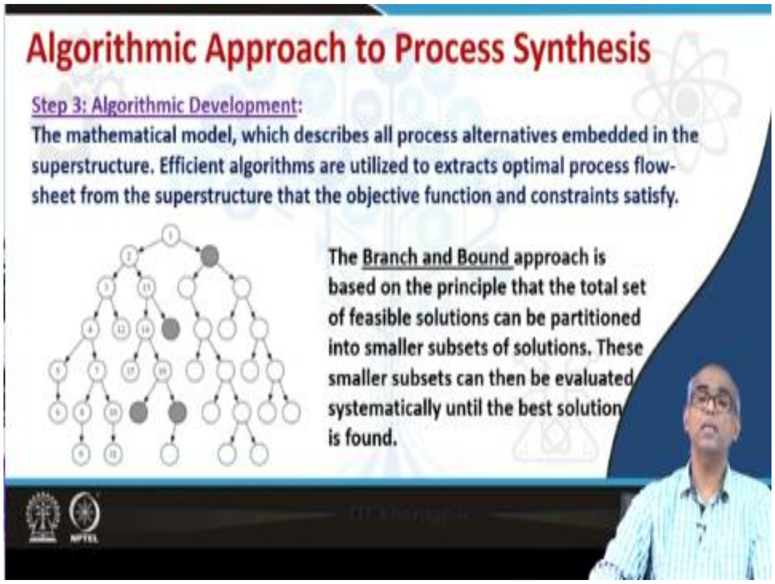

Algorithmic Approach to Process Synthesis

Step 3: Algorithmic Development:

The mathematical model, which describes all process alternatives embedded in the superstructure. Efficient algorithms are utilized to extracts optimal process flow-sheet from the superstructure that the objective function and constraints satisfy.

The Branch and Bound approach is based on the principle that the total set of feasible solutions can be partitioned into smaller subsets of solutions. These smaller subsets can then be evaluated systematically until the best solution is found.

Now second we need to have a proper algorithm to solve such mixed integer nonlinear programming problem. Now the branch and bound method is widely used. The branch and bound approach is based on the principle that the total set of feasible solutions can be partitioned into smaller subsets of solutions. These smaller substance can then be evaluated systematically until the base solution is found.

So you have representations of superstructure, then the formulation of mathematical optimization problem which is generally a mixed integer nonlinear programming problem and then an algorithm to solve such problem, which is generally a branch and brown method.

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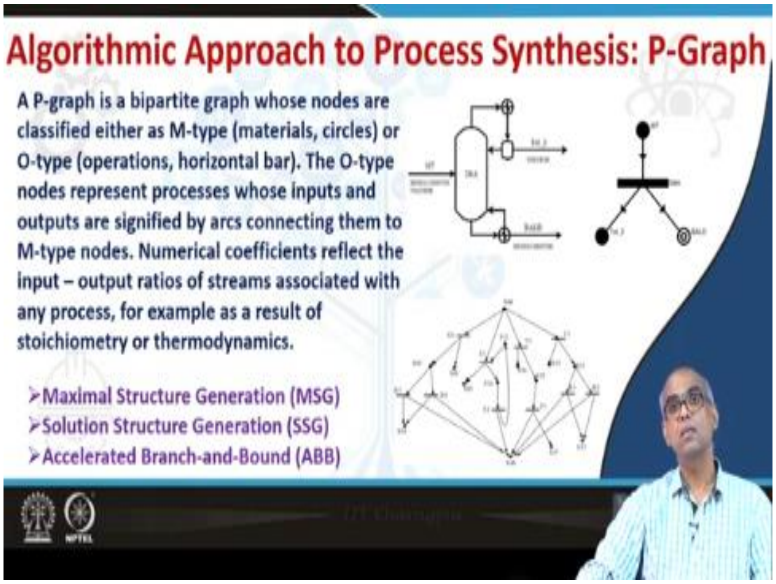

## Algorithmic Approach to Process Synthesis: P-Graph

A P-graph is a bipartite graph whose nodes are classified either as M-type (materials, circles) or O-type (operations, horizontal bar). The O-type nodes represent processes whose inputs and outputs are signified by arcs connecting them to M-type nodes. Numerical coefficients reflect the input – output ratios of streams associated with any process, for example as a result of stoichiometry or thermodynamics.

- ➢Maximal Structure Generation (MSG)
- ➢Solution Structure Generation (SSG)
- ➢Accelerated Branch-and-Bound (ABB)

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A P graph or a process graph is frequently used for such process synthesis problems. A P graph is a bipartite graph whose nodes are classified as either M type that is material stack which are this circles or O type which are these horizontal bar which represents operations. So a P graph is a bipartite graph which contains of two types of nodes M types and O types. M types are circles which represents materials and O types are horizontal bars, which represents operations.

So the O type nodes represent processes whose inputs and outputs are signified by arcs connecting them to M types nodes. Numerical coefficients reflect, the input output ratios of streams associated with any process, for example as a result of stoichiometry or thermodynamics. See this is a distillation column where benzene and toluene is being separated.

Toluene is taken out a top product, benzene dehydrate is taken out as bottom product. So this is a conventional representation whereas this is representation in terms of P graph. Note that this is Pm 7. So this stream this is represents this is material M type node, whereas this horizontal bar represents this distillation operation. So two streams comes out one material stream toluene, another material stream, is this benzene dehydrate.

Now, so now there are 3 algorithms which will be used on these P graphs and the base flow should be obtained. First is maximal structure generation MSG it is nothing but a way to obtain the superstructure which will consist of this P graphs. So a very very simple example may be this. A superstructure for a reasonable problem will be much more complicated than this. Then solutions structure generation, this is the another algorithm which will give you a subset of maximum structure.

This will be the combinatory feasible solutions, so this is a subset of what you get from maximum structure generation and then the branch and bound algorithm in particular accelerated branch and bound algorithm to obtain the best or the optimal flow sheet from this feasible flow sheets that you obtain using solution structure generation. So maximum structure generation algorithm, solutions structure generation algorithms and accelerated branch and bound algorithms are systematically applied to obtain the optimal flow sheet through algorithmic process.

With this we stop our discussion on this module. So what we learnt is essentially the hierarchical approach to process synthesis, we have discussed in very details and we have very very briefly outlined the algorithmic approach to process synthesis.