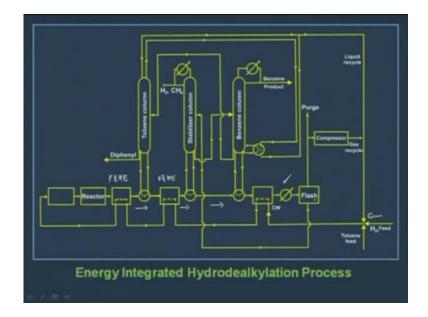
Process Design Decisions and Project Economics Prof. Dr. V. S. Moholkar Department of Chemical Engineering Indian Institute of Technology, Guwahati

Module - 1 Nature of Process Synthesis and Analysis Lecture - 3 Hierarchical Approach to Process Design – Examples

Welcome, today we shall see the hierarchical approach to process design. But before I do that, let me give a brief recap of what we learnt in the previous lecture. In previous lecture, we learnt about the nature of process synthesis, the steps involved in the synthesis, we saw how process synthesis is a creative activity; it is an art coupled with a technology.

And then we saw how we can design a very simple flow sheet based on the chemistry of the process. We took the case study of hydro dealkylation of toluene and then we drew a very simple flow sheet for the process. The reactions involved where toluene reacts with hydrogen to generate benzene and methane. And there is a side reaction that benzene undergoes 2 moles of benzene combined to give one mole of diphenyl and hydrogen. So, diphenyl is the side product of the reactor of the process and benzene is the main product.

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Then I showed you the actual flow sheet of the process; which now you see on the screen. Now, this flow sheet is an energy integrated process, which means that we not only couple the process units, reactor, distillation columns, flash drum, vapor recovery systems so on and so forth. But we also try to recover the energy of the streams hot streams into those require to be heated. For example, the reactor affluent is at very high temperature something like 845 Kelvin. And we cool it in different steps to see on the screen; this is a feed to affluent heat exchanger, this is another feed to affluent heat exchanger; where we try to heat the incoming feed with the outgoing stream from the reactor. We also tried to drive the reboiler of the 3 columns using the heat of the affluent stream that is emerging from the reactor.

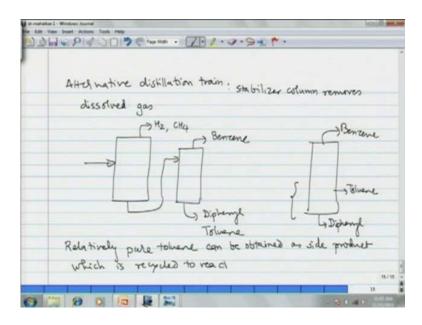
And, finally the remainder heat is taken out in this heat exchanger; the one which is shown by tick mark. And then the stream pressure is reduced, the stream is flashed which gives the space split. But before we can arrive at such a complicated flow sheet; we need know lot of things almost all the flow sheet like for example, we need to know the molar flow rates of all the streams, we need to know the heat capacities, we need to know the temperature so on and so forth. So, obviously the heat integration of the process is the last step in process design; when we have designed the entire flow sheet. So, we start with a simpler version; now, how do we start?

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Let us first focus our attention to the distillation train that are there. The reactor affluent comprises of 5 products; these are the main product benzene, the side product diphenyl, unreacted toluene the reactant; then hydrogen and methane. Now, in the flash drum 3 out of these products condense. For example, like benzene diphenyl toluene condense into liquid which is now then sent to distillation train.

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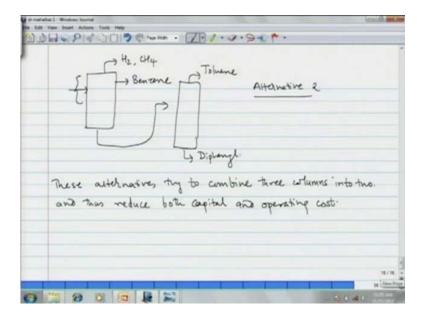


Now, the distillation train comprises of 2 columns, 2 main columns essentially; first column to take off the main product benzene and second to distill off the diphenyl which is a side product from the unreacted reactant. But the question arises is it necessary to have 2 columns to withdraw 3 products; we can combine some of these columns. Now, let us see a process alternative; the liquid that comes out of the flash drum contains lot of dissolved gas both methane and hydrogen are dissolved. So, before this liquid is sent to main distillation train; this dissolved gas has to be taken off and that job is done by the stabilizer column. So, we note that point that stabilizer column removes dissolved gas.

So, we have a simple flow sheet; first column stabilizer column taking of the gases, and then the liquid stream going to the next column, where benzene is removed as a top product and diphenyl and toluene is removed as bottom product. However, diphenyl is much lesser in quantity as compared to toluene. Now, we shall see this in the material balance for the process; that we will take up in the future lectures. And it also the composition of this of the distillated bottoms also depends on relative volatility; it is possible to take off toluene as a side stream.

So, the second column can be modified as benzene as a distillated product, and toluene as a side stream from one of the plates near the bottom; and diphenyl as a bottom product. Now, how is this possible? The relative volatility between toluene and is quite high diphenyl is quite high. So, if you look at the bottom plates of the distillation column; the composition changes very fast like bottom is almost pure diphenyl. And the quantity of diphenyl in the upper plates is relatively small.

So, if you take off toluene as a side stream from one of the plates near the re boiler. Then you can obtain relatively pure toluene that point we note; that relatively pure toluene can be obtained as a side product; this toluene may not be 99 percent pure. But this toluene is being recycled to the reactor; it is not a product. So, we can compromise with the purity of toluene; relatively pure toluene can be obtained as side product which is recycled to the reactor. This is possible only if diphenyl is present in small quantities; and relative volatility between toluene and diphenyl is high, that point should also be noted.



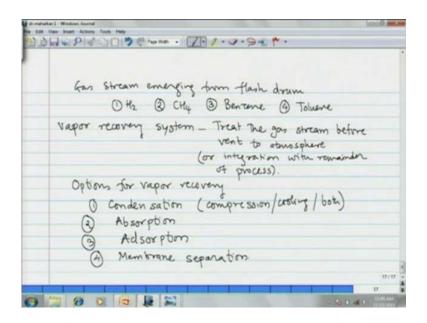
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Another option is to take off benzene as a side product from the first column; the stabilizer column itself. And then send the stream to the second column; where the toluene and diphenyl are separated this is alternative 2. Now, how is this possible; hydrogen and methane being gases are can be separated from toluene vary from benzene

and toluene very easily. So, if you see the composition of the topmost plates; in the first column you see very rapid change of composition the near the topmost plate benzene will be almost pure. And you can withdraw benzene as a side product from the first column. So, essentially with these alternatives we combine 3columns into 2 columns; these alternatives that point you note; the alternatives try to combine 3 columns into 2; and thus reduce both capital and operating cost.

Now, which of the alternatives is better? Well, that depends on various factors that for example, what is the conversion obtained in the reactor, what is the molar composition of the feed streams so on and so forth? So, the distillation column can be designed only after we know the composition of reactor affluent; for which we need to design the reactor itself. So, we put the design of the separation system as an activity before we do heat integration; that is second last activity. Now, this is about separation of liquid streams.

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Flash drum also gives rise to a gas stream. And that stream essentially is hydrogen, methane plus some vapor of benzene and toluene that point we note; that gas stream emerging from flash drum has 4 components; hydrogen, methane and some vapor of benzene and toluene. Now, benzene is carcinogenic so we cannot have emission of benzene from the process. And benzene is also a valuable product that we need to recover; using benzene is going to hamper the economy of the process. So, we have to

design a vapor recovery system that will treat the gas stream before it is vent to atmosphere. Now, the gas stream that is emerging from the vapor recovery system need not always be vented to atmosphere. In the present context we have hydrogen and methane; both of which can form fuel. So, this stream can be recycled in the process to meet the energy demands. So, that point also we note that before went to atmosphere or integration with the remainder of the process.

Now, if you have to remove a vapor from gas we have several options. In the first place we need to know as how we distinguish vapor from gas; gas essentially a vapor which is far removed from a critical point. For example, hydrogen, methane, nitrogen, oxygen are gases but benzene and toluene can be characterized as vapors. Because these can these are not far removed from their critical point; and these can be condensed with relatively less effort. So, to recover these vapors we have several options; one obvious option is that of condensation. We can condense vapor by compression of the stream or cooling of the stream or both simultaneously.

Now, whether the vapor will condense with simple compression or we need to apply cooling as well depends on the p v t characteristics of the vapor. For example, propylene can be condensed by compression to moderate pressure something like 8 to 10 bar using cooling water that is all. The second option for recovery of vapor will be the tough absorption in a suitable solvent. The third option is that of adsorption on a suitable adsorbent; and fourth option is the membrane separation.

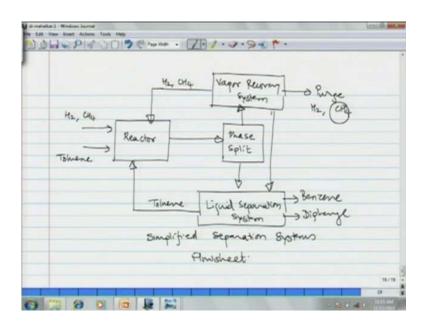
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Now, first decision that we have to make is that each the vapor recovery system needed. And if it is needed; what is the economy of vapor recovery? Before, we choose the process for vapor recovery; we have to realize that a vapor recovery system may cause an additional load on the liquid separation system; because let us say the choice of absorption. Absorption is a well established operation for dilute compositions of gas; absorption is the most economic operation as have been proved in several studies. However, absorption will need a solvent and the solute has to be recovered from the solvent through distillation or something like stream stripping. And therefore we have to take into consideration the economics of the process; before we design the vapor recovery system. Now, we are going to see a case study of design of vapor recovery system in coupled with economics.

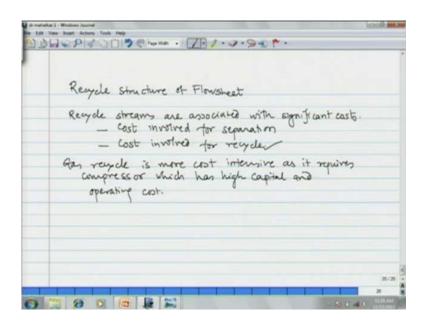
So, we leave this point and take up the next; that is the simplified flow sheet of separation system. The separation system components are a flash drum, a liquid separation system which contains distillation columns, extraction units, even membrane systems so on and so forth; and then the vapor recovery system which may contain absorption, adsorption or membrane processes. Now, if I have to draw a simplified flow sheet of the process including the separation system.

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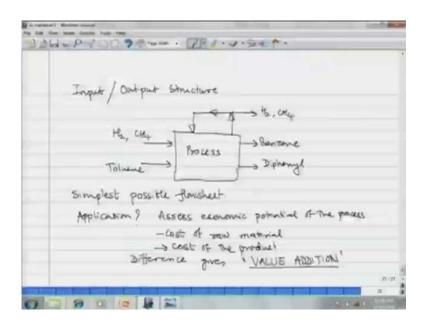
Then, we can draw the reactor with feed streams of hydrogen and methane, toluene; the reactor affluent goes for phase split. Phase split could be obtained by reducing the pressure or cooling or both; and then phase split will give rise to 2 streams a gas stream from which vapor has to be recovered and a liquids separation system. From liquid separation system products and byproducts will come out; and the unreacted reactant is sent back which is toluene. Similarly, from vapor recovery system the gas stream will emerge. Now, some of these gas is purged in order to limit the concentration of the innards which is methane in the process and rest is recycled. So, what you see now is the simplified flow sheet. However, we must also know that the vapor recovery system will give rise to the liquid stream; that needs to be treated in the liquid separation system for the recovery of solute. So, what you see is the simplified flow sheet of the separation system.

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Now, we talk of recycling both gas and liquid. So, the recycle structure of flow sheet comes next; why do we have to consider the recycle structure separating? Because recycle streams are associated with significant cost; the cost involved separation of the unreacted reactant and the cost involved for recycle. Now, as far as the second cost is concerned cost for the recycle this cost is not much for liquid streams. Because liquid can be simply pumped and cost of pump is very small is a minor item in the process flow sheet. However, if we have to recycle gas then we need a compressor which is not only cost intensively in terms of capital cost also the operating cost. So, the gas recycle is more cost intensive as it requires a compressor which has high capital as well as operating cost.

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Now, to further simplify the flow sheet we draw the input, output structure; which means that we simply draw a box and show the streams that go into the process and that emerge from process. Now, here we do not show the recycle of toluene; because it is an internal process. So, this is the input, output structure flow sheet which is the simplest possible flow sheet of the process. Now, what is the use of such a flow sheet; that a question may arise in your mind very quickly? We need to study the input output structure of flow sheet; in order to assess the economic potential of the process; what is the cost of raw material and what is the cost of the products? The difference between these will give the value addition. So, the input output structure helps us to determine a very crucial parameter of process design that is a value addition.

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Sys	tematic Approach for Process Design
	* Assessment of economic potential at each step
	-) AltoLnatives of process design
H	ierarchy of Decisions for Process Design
	Batch or Continuous process
2	Input/out put structure of flowsheet
	Recycle structure of flowsheet
6	Segaration system - Vapor secovery

Now, if we design a process from input, output structure then to recycle structure then to separation system. And then to energy integration what we have is a very systematic approach for process design. Now, this approach gives us an estimate of the economic potential from step to step; as we include more and more effort to design a process to rigorous extent; we have to assess whether these efforts are worth. We will also come to know with this approach what are the alternatives for the process like when we considered the design of distribution columns we could immediately take out 2 process alternatives. Another process alternative is not to recycle diphenyl, to recover it as a product; an option will be to recycle diphenyl to extinction. So, that it builds up in the process and since it is a reversible product it remains at a particular concentration.

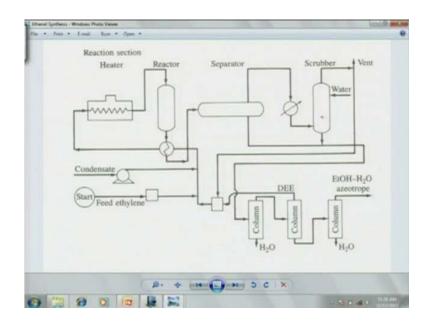
So, with this systematic approach for process design we not only get an idea of the economic potential at each and every steps of process design. But we also generate the alternatives of process design. So, the hierarchy of decision for process design has 5 steps; the first is determine whether you want to go for a batch or continuous process. Then next determine the input output structure of flow sheet which will give you the value addition of the process; and whether the cost of operation is worth the value addition. Then comes the recycle structure of the flow sheet then comes the design of the separation system. And in this we saw 2 separation systems; the vapor recovery system and liquid separation and finally comes the heat integration.

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Now, we shall see another example of designing of flow sheet step by step method like basically an application of hierarchy of decisions that we just listed ok. And we shall see now example of ethanol synthesis. Now, ethanol is manufactured by hydration of ethylene; the chemistry of the process is as follows ethanol plus H 2 O giving reversibly sorry, I am sorry this is ethylene hydration ethylene plus H 2 O gives ethanol. And 2 molecules of ethanol reversibly combine to give diethyl ether and water as side product.

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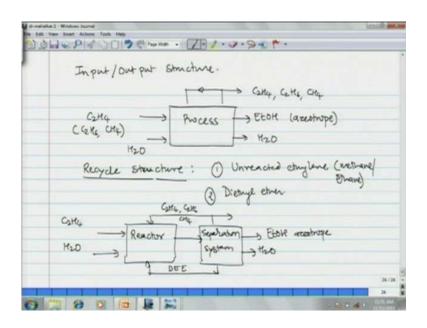
Now, what you see on the screen is again a complete heat integrated process with recycle streams and everything for ethanol synthesis. So, the fresh stream of ethanol enters then it undergoes it is mixed with the condensed process. And then it goes for heating then it enters the reactor; and then a separator and then we have 4 columns 1, 2, 3, 4 to separate the products.

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EXAMPLE: ETHANOL SYNTHESIS			
Clamistry: Ethylane + 120 = 1	Elhanu	{	
2 Ethanol 1 D			0
Reaction Condition: Temp Stok prescure 69 6			
Single pass conversion: 7%. Etuglen Equilibrium constant for DEE		-7	
Feed streams: Pure walk Ethylene streams			
- (C2H6 Mothane	
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Now, the reactions conditions are 560 temperature of 560 Kelvin and pressure of 69 bar. Now, in single pass conversion 7 percent of ethylene reacts; the equilibrium constant for diethyl ether; that we abbreviate as DEE is K approximately equal to 0.2 at reaction condition; the feed streams for the process are pure water and ethylene stream that contains 90 percent ethylene, 8 percent ethane and 2 percent methane. And based on the energy integrated flow sheet we have now; we have to design now the hierarchy of decisions.

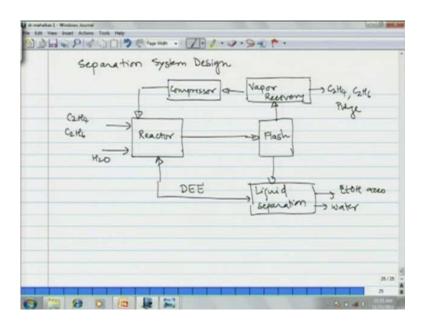
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Now, let us first input output structure of flow sheet. If we draw a box and the feed streams going in which is ethylene with some impurities of ethane and methane and water? The output streams are ethanol but in the form of an azeotrope and water; and unreacted ethylene is recycled. And a part of it is purged to keep the level of impurities ethane and ethane and ethane and methane under limit. So, what you see here is a input output structure of flow sheet which is simple as possible.

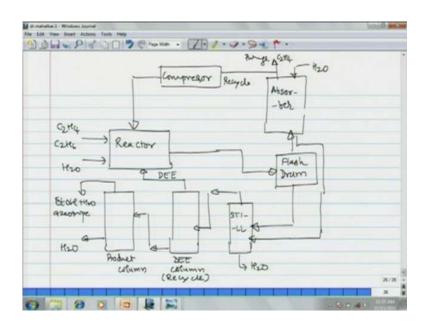
Now, let try to design the next step; the recycle structure of flow sheet. But before we do that we have to see what are the components, that are recycled? The recycled components are unreacted ethylene with impurities of methane and ethane, and second is the diethyl ether. Now, with this we can draw a simple recycle flow sheet as the reactor in which the feed stream enter. And then a separation system from which the main product emerge ethanol azeotrope and water, and then the liquid recycle stream contains diethyl ether and gas recycle stream is ethylene and the impurities.

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Now, we go for the separation system design or the general structure of the separation system. Here, we can draw a reactor with feed streams. Now, the reactor affluent is first flashed; flash drum gives rise to 2 streams; first is the vapor recovery system from which 2 streams emerge the purge stream and the recycle stream. However, before we recycle the stream we have to put a compressor that will restore the pressure of the stream to 69 bar. So, this is a general structure of the vapor recovery system. Similarly, we can design, we can draw a liquid separation system from which ethanol azeotrope and water emerge as product; and diethyl ether is the recycle stream. So, what you see on the screen is the general structure of the separation system.

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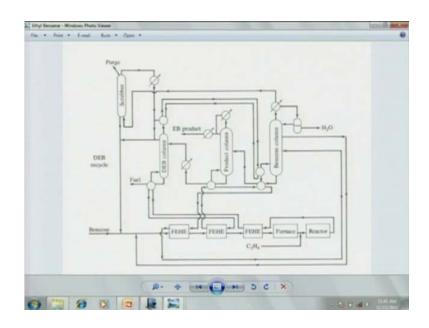


Now, the next step is to expand the sections corresponding to vapor recovery system and liquid separation system. Now, as you see in the integrated flow sheet; the vapor recovery system comprises of an absorber. Under liquid separation system comprises of 3 displacing columns. Now, we try to organize these units in the form of a block diagram. First we draw a reactor with feed streams ((Refer Time: 39:53)); then comes the flash drum, the gas stream emerging from the flash drum is admitted into an absorber in which water is used as a solvent the streams emerging from absorber are split into purge. And recycle stream is obviously compressed before it is admitted into the reactor.

Now, for the distillation column we have 3 units; column one which takes off water. Now, we can also admit the water emerging from absorber into this column. This is essentially a steel which mixes the streams; the output of this steel will go into the first column which is the diethyl ether or the recycle column. Here, the reversible product diethyl ether will be taken out and will be recycled into the reactor. The bottoms of this column will be admitted to the third column which is the product column; from which the main product ethanol plus water azeotrope will emerge as the main product. And some water will come out which could again sent back to the reactor. So, what you see on the screen now is the complete blocked diagram of the process ok.

So, this is how you can decompose a complete flow sheet into simper flow sheet; where you can make hierarchy of decisions for the process design. The first that we saw was input output structure; then the recycle structure, then the general separation system and then the complete design. Now, we shall see another example of a similar kind where we will develop the hierarchy of flow sheets; the problem that we take now is that of manufacture of ethyl benzene.

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Now, what you see on the screen is a complete heat integrated process for manufacture of ethyl benzene using ethylene and benzene as raw materials.

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Dele Port COS Come . Z. 1. J. 9. EXAMPLE 2: Manufacture of Ethyl Bonzone (Hierarchy of Flowsheets) Chemistry Etnylane + Bentene -> Etnyl barrene (23) Ethylene + EB = Diethyle benance (DES) Ethylene + DEB = Trietnyl benane (TES) 2 Ethyl tencene 2 Benzene Pressure= 300 peg -> Reaction condition Ten 820'F Cat yeach m reaction runs with excess of bonzene to complete conversion of etypone enforce (to 0 10 1 1 0

But let us first see what is the chemistry of the process? The main reaction is ethylene reacting with benzene to yield ethyl benzene as the main product. Now, we will use abbreviations as EB. Now, there are 2 side reactions that also occur; ethylene further reacts with ethyl benzene. And this reaction reversible to yield diethyl benzene; and diethyl benzene further undergoes reaction to yield triethyl benzene. Now, the third reaction is also reversible. Moreover 2 molecules of ethyl benzene can combine reversibly to give benzene plus diethyl benzene. The reaction conditions are temperature of 820 degrees Fahrenheit and pressure of 300 psi gauge and it is a catalytic reaction. Now, the reaction runs excess of benzene to enforce complete conversion of ethylene. Now, the rational is also to suppress DEB and TEB formation which are unwanted side products.

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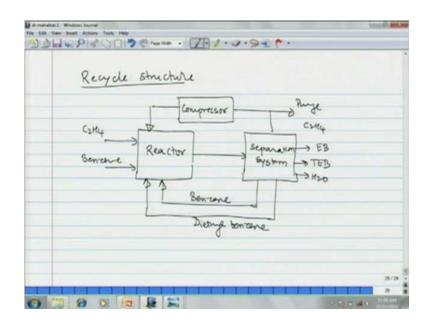
Feed streams: Benzane (0.28% walter impurity) Ethylene (1% ethane) Two reactors - one on the stream seemd regeneration for coke formation Input/Dutput structure (2144 (2144 (3244) hocess - EB to TEB to TEB to TEB to TEB		10 7 C 14 mm	· Z• .	9.94 r.		-
Input/Dutput structure (244 (344) houss 5EB barrane (H20)	Feed		Bencone Ethylone	(0.28% usalia (1% emane)	impurity)	
Input/Dutput structure (244 (344) houss 5EB barrane (H20)	Two	reactors	one on D seemd n	re stream egeneration for	coke format	in
(GH) houss SEB binnene borro (H2O)	Inp	wt/Output	structure			
(H2O)		((2H4)	houss .			
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The feed streams for the process are benzene which has 0.28 percent of water as impurity. And ethylene which has about 1 percent ethane as impurity; usually for this process 2 reactors are used, one on the stream and second we just kept for regeneration due to coke formation. And now we have to design the hierarchy of flow sheets for this process. We just saw the energy integrated version of this; you can see that the benzene enters it is heated through 3 FAG which is feed to affluent heat exchangers; before entering a furnace which gives the remaining heat. And then it enters the reactor the reactor affluent exchanges heat with the incoming feed in 3 exchangers; first exchangers then it drives the reboiler of diethyl benzene column; then it again enters the heat

exchanger for feed. And then the emergence stream dives the reboiler of the product column and again it enters. And then finally it drives the feed of the reboiler of benzene column ok.

Now, we have to design the simpler flow sheets for this complicated design. So, let us first design the input output structure of the flow sheet. As you will see in the in the flow sheet the diethyl benzene is recycled into the process. However, the triethyl benzene which is the bottom product of the diethyl benzene column is take out and used as a fuel. So, for this process there are 2 feed streams; first ethylene with impurity of ethane and benzene with impurity of water. The out coming streams are the main product ethyl benzene, the side product triethyl benzene which is further used as a fuel in the process and water. And secondly the unreacted ethylene is also recycled in the process. So, what you see now is the simplest structure of the complicated flow sheet; we have decomposed the flow sheet into a simple blocks which shows only the input and output streams.

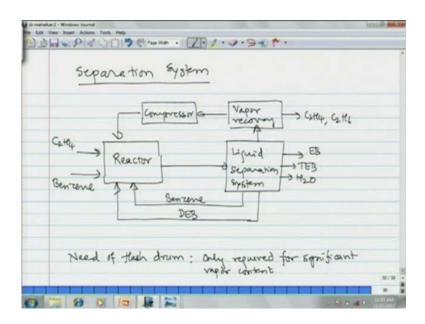
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Now, we go a step further to design the recycle structure of the flow sheet. Now, as we see in the energy integrated process there are 2 streams that are recycled; 2 liquid streams that are recycled. First stream is that of unreacted benzene and second stream is that of diethyl benzene. So, we now draw a reactor with input feed streams; then the separation system as a box. Separation system comprises of both vapor recovery and liquid recycle

and then 2 liquid recycle streams emerging one for benzene and another for diethyl benzene the product streams that remain same ethyl benzene, triethyl benzene, water. And then the purge and recycle stream for gas; like in previous stream we have to restore the pressure of the recycle stream, gas recycle stream through a compressor. So, what you see now is a simplified recycled structure of the flow sheet.

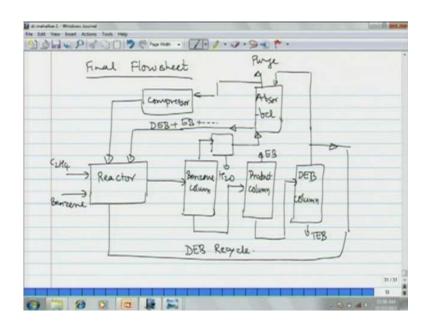
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Now, the next stage is to design the separation systems flow sheet; in which we open the separation system box. And show the liquid and vapor recovery systems separately; the earlier structure of the flow sheet remains the same. We have reactor then the reactor affluent goes in a liquid separation system from which the product streams emerge; the main product ethyl benzene, side product tri ethyl benzene and water. Now, you may ask that why did we not consider a flash drum before a reactor as we have considered in the 2 previous process. Now, need of the flash drum depends on the vapor content of the of the stream that is emerging from the process and also the p v t characteristics. If by simple pulling the products condense then we do not need a liquid separation system.

Then, we have vapor recovery system; which gives rise to purge and recycle streams. In the recycle we have a compressor that we had shown earlier under. And for the liquid separation system we have 2 products that are recycled benzene and diethyl benzene. And finally we give the structure of the flow sheet where we elaborate on the liquid separation system.

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Now, here we show all the units that are in the process, all the major units that are in the process; the reactor with feed streams. Then the reactor affluent that goes to benzene column; the first unit in the separation system, the output of benzene column goes to the products column where we take off ethyl benzene the main product of the process. Then we sent the stream to diethyl benzene column; where we take off the side product triethyl benzene. And send it to fuel the distilled product of diethyl benzene column is split in 2 parts; one part is recycled to the reactor. And the second part is used as liquid in the absorber that treats the un-reacted ethylene stream that is emerging from the process. Now, ethylene is taken out from benzene column itself and admitted into the absorber. And from absorber 2 streams emerge; the purge stream and then the recycle stream for gas and it is compressed before admitting into the reactor.

Now, the liquid that emerges from the absorber could also go to the reactor. Because it contains mostly diethyl benzene plus some ethyl benzene and plus other product. So, what you see here is now a complete flow sheet for the ethyl benzene manufacture as a block diagram. In the next lecture we shall see the first decision in detail; that is to decide whether we have to design a process in batch or in continuous mode. And what are the governing factors for this decision?