Mathematical Modelling and Simulation of Chemical Engineering Process

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Lecture 05

Process diagrams

Hello everyone and welcome to the last lecture of this first week. Here today we are going to talk about some of the process flow diagrams, that we generally encounter in Chemical Engineering Systems as these are very, very important and we are also going to talk about different considerations that needs to be satisfied or you need to keep it in mind while trying to design a process flow sheet.

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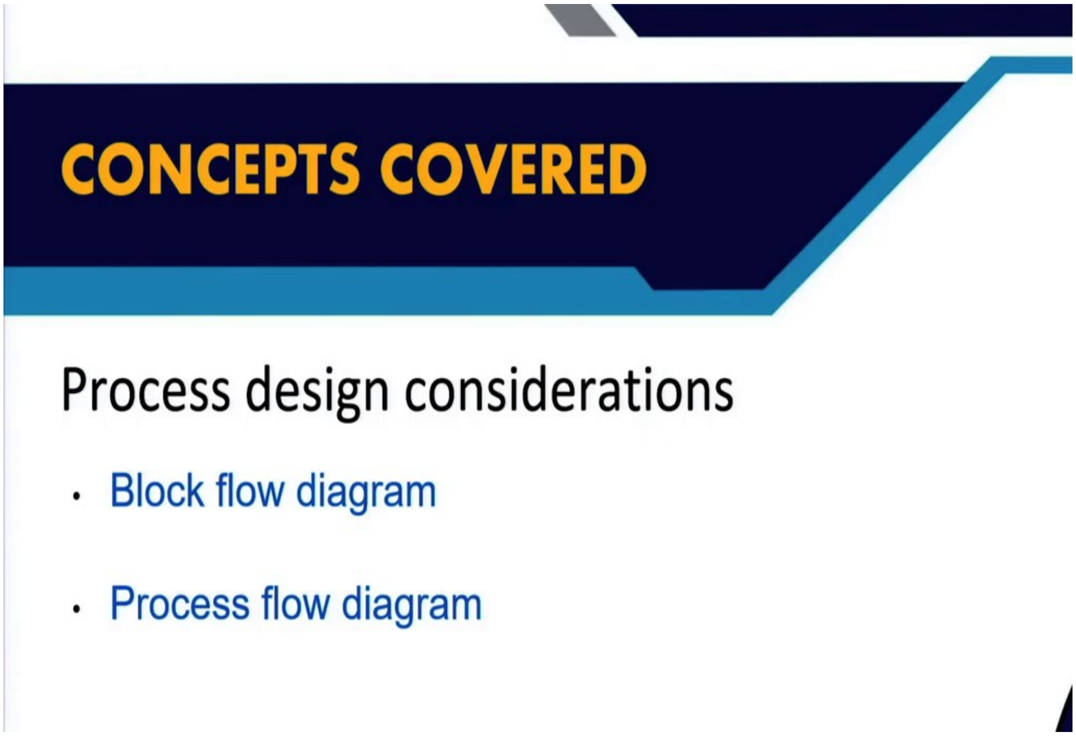

CONCEPTS COVERED

Process design considerations

- Block flow diagram
- Process flow diagram

So, let us start. As you know that process diagrams are generally of three types, block flow diagram, BFD, these are called BFD, then you have the process flow diagram, PFD and then you have the piping and instrumentation diagram. So, we are skipping this piping and instrumentation because that is mostly a part of our different course. And here I just want to give you some idea and some thoughts on how do you design such sheets and how do you can arrange or how you can (yes) arrange the different units in a plant.

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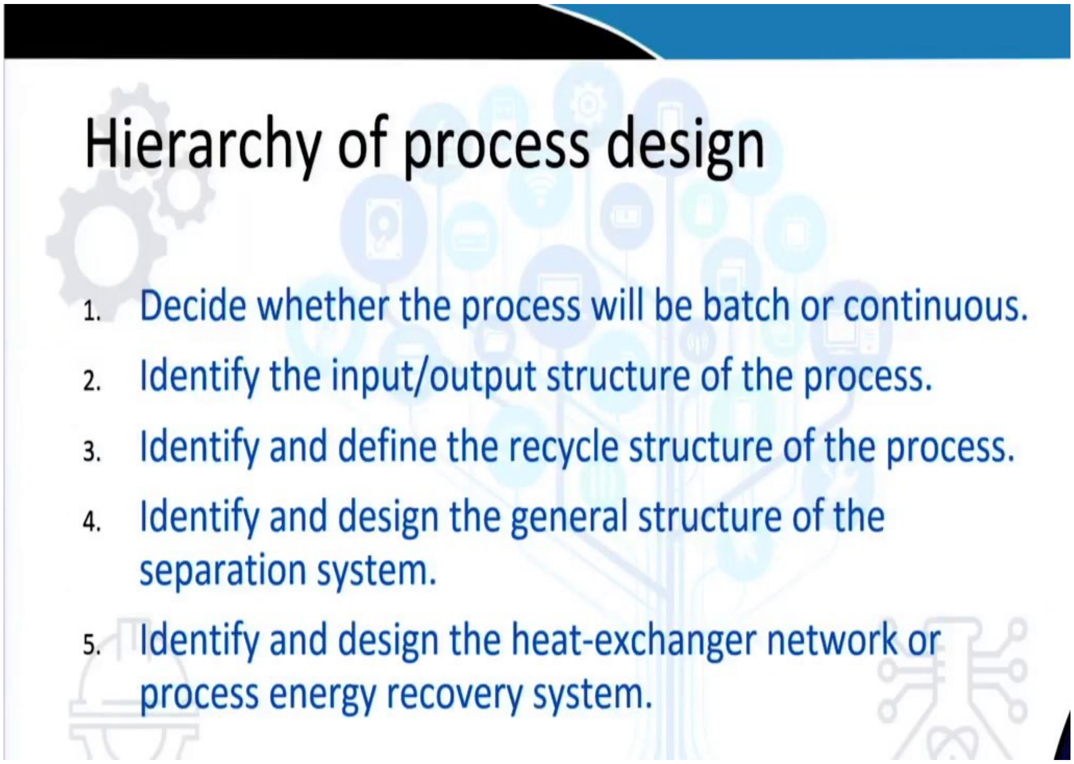

Hierarchy of process design

1. Decide whether the process will be batch or continuous.
2. Identify the input/output structure of the process.
3. Identify and define the recycle structure of the process.
4. Identify and design the general structure of the separation system.
5. Identify and design the heat-exchanger network or process energy recovery system.

So, the hierarchy tells you in the process, is that these are some of the five thumb rules that is very critical to be decided before you design a process or before you design a plan. First thing is whether the process will be batch or continuous, this is one of the most critical decision that needs to be taken.

Often this depends from two criteria is that the scale of the system and second is the economics. And the second part or the second important thing is that you need to identify what are the, what would be the input and the output structure of the process. Whether do you need any additional processing units in the downstream or in the upstream that needs to be defined or that needs to be decided then is the recycle structure.

So, almost all chemical engineering processes would need some sort of recycle, so, as to reuse the particularly the component which was like unused or remain (not was) not fully converted. So, this recycling is very important. So, you need to consider the recycling. The fourth important point is to identify that separation system. So, whether it is a gas-liquid product system or whether it is multiple components system? whether you need single units or multiple units? whether there are environmental considerations? for which additional separation units needs to be there.

And finally, is that energy optimization or the energy recovery system what should be the heat exchanger network or if there are any wasted recovery system that you need to implement. Now, please note that these five considerations should be decided in a sequence, and this is the sequence. So, you cannot decide I mean should not decide first on the heat extender network, and then you decide whether you want a better a continuous process. So, the sequence of the design components has to be kept in mind and this is like the general heuristics for process engineers.

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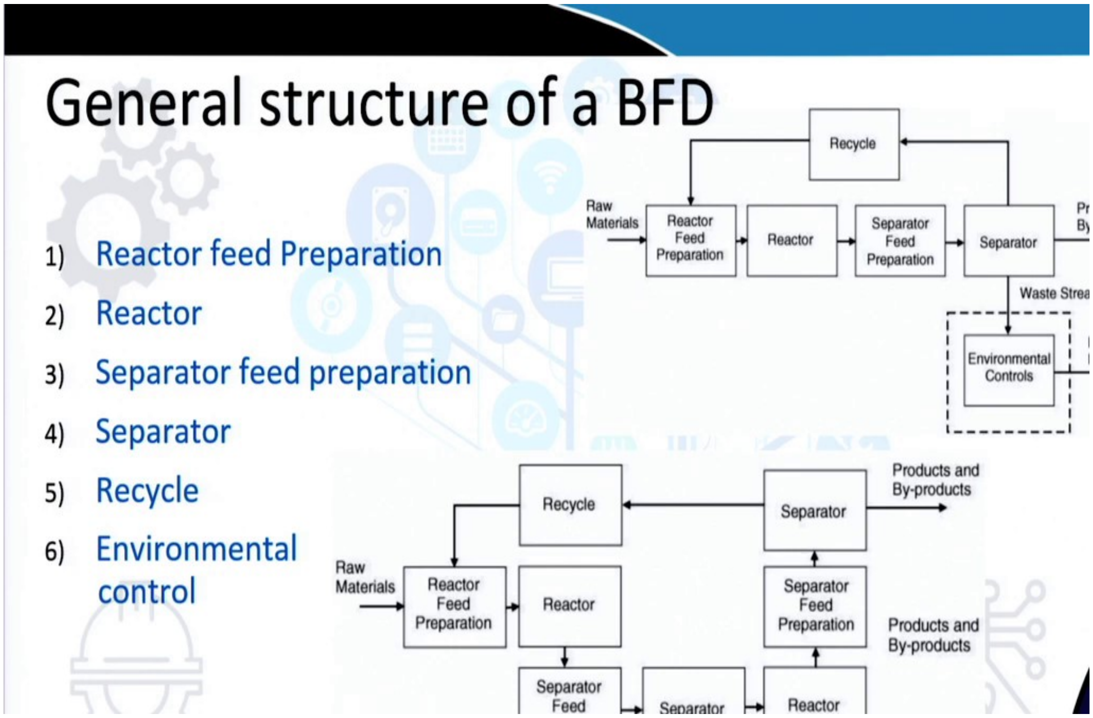

General structure of a BFD

1) Reactor feed Preparation
2) Reactor
3) Separator feed preparation
4) Separator
5) Recycle
6) Environmental control

Now, coming to the general structure of a block flow diagram, as you can see, it has essentially six components. First is the part related to so, ultimately in a process we want our raw materials to be converted to the desired product and it goes through a series of units. So, what are the important components or the structure: one of them is the reactor feed preparation then we have the reactors then we have the separators or the separator feed preparation before we try to have the separator in place, and then the recycled stream and then the environmental control or the environmental protocols if something is there that needs to be satisfied.

Now, interestingly the feed chemicals generally, so, coming into each one of them step by step that the feed chemicals generally come from a storage. So, before they are fed to the reactor, like the reactor there are some certain reaction conditions. It is often required that the feed should be either pre heated or it should be pressurized and bring it to the appropriate or close to the conditions of the reactor before it is fed into the reactor otherwise what will happen there will be a big fluctuation in the process variable, due to the sudden change in the process condition of a untreated or unprepared feed. So, the reactor feed preparation is very, very important.

The second part is the reactor, which is one of the heart of the process and all the important desired products form in the reactor, there are formation of byproducts too. So, the reactor is the place where you actually have this mixing of the cooking of the raw materials. Now, there are important questions which needs to be asked for, before you think of the reactor. First thing is that at what phase that the reaction takes place, whether it is the liquid phase, vapor phase or the mixed phase ? So, the answer will help you to decide what should be the related feed preparation as well as the type of the reactor. So, if there is a vapor phase then it is very essential that the whatever the feed that you are getting to the reactor should be in a vapor state in the upstream. The next is what is the required temperature and the pressure in the reactor.

So, if it is a very high pressure or a high temperature process then also it there needs to be some pretreatment to the feed. So, the thumb rule says that if the reactor feed temperature is more than 250, sorry more than 150 degrees centigrade, then essentially a fired heater or a feed preparation unit for raising the temperature is very, very essential.

Whether this reaction is equilibrium controlled or kinetically controlled ? So, general equilibrium reactors are large in size but cannot be controlled reactors can be smaller. So, majority of the gas phase or liquid phase reactions are generally kinetically controlled. So, that is something you need to consider. Another important is that what is the per-pass conversion. So, if it is an equilibrium reactor, you need to have a high per-pass conversion. So, then again this brings to the mind that how this conversion efficiency can be increased what sort of catalyst is required, whether it is solid catalyst, whether it should be homogeneous, whether it needs additional promoters ?

So, these are the questions that comes to the mind. The other important factors to be kept in the reactor design is whether the reaction is exothermic? Endothermic? how do you control the temperature? how much is the heat change or the exothermic heat this heat release or the endothermic heat requirements and what sort of cooling water requirements are needed?

What is the selectivity of the desired reaction? How much is the unwanted components in the in the reactor? will play a role or will influence the reaction state. What would be, here is another important question generally for gas phase reaction, what would be the possibility that the reactor feed or the products present would reach explosive limits? and this is particularly true for the case of hydrocarbon based reactions.

So, these are some of the important criteria that needs to be kept in mind when thinking about the reactor. Regarding the separator, the general idea that comes to the mind in the case of separator is that: is the separation I mean separation of the unwanted undesired components, what is the cost involved? and what sort of purity are we looking into the final product? So, the separation or the separation units are generally dependent on the price or on the cost or economics involved in the purity of the product.

So, whether additional stages or additional units are required to achieve certain level of purity? Does the presence of these impurity somewhat destabilizes our product? The another important question that comes is that what is the amount or the impurity in hazardous they have an environmental issues on the product? So, in general you have to determine what is the minimum number of the separation units that is needed for the process?

So, if you have, so, generally our process would be having one, I mean a separator would be having one inlet stream and two outlet stream. So, you would be needing, so, you will be needing n minus one units for n outlet streams that is the general thumb rule, isn't it? So, that is how you are going to think about a plan about your separator.

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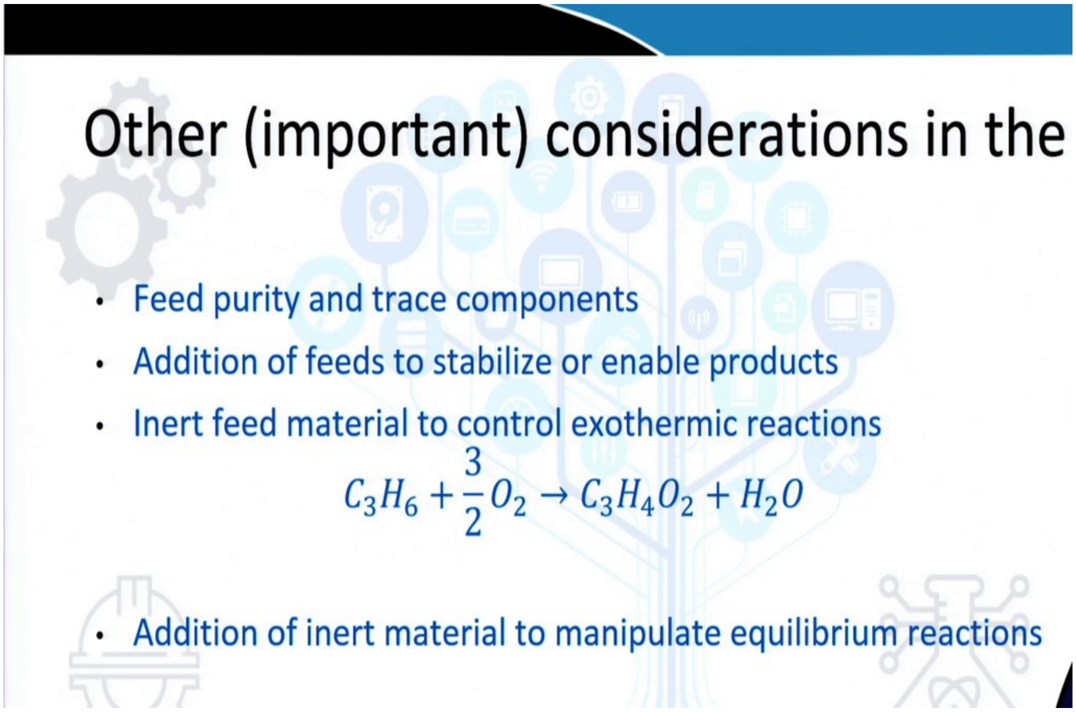

Other (important) considerations in the

- Feed purity and trace components
- Addition of feeds to stabilize or enable products
- Inert feed material to control exothermic reactions

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O$$

- Addition of inert material to manipulate equilibrium reactions

So, another important consideration in the process is the feed purity and the trace components. So, generally the feed purity when we talk about the feed purity, it is very essential to understand that whether these impurities present in the feed at all contribute, at all contribute towards the I mean, do they take part in the reaction? if it is yes, then these needs to be definitely removed.

Next question is how what is the fraction of these in these impurities, if they are presenting large quantities let us say 10 to 20 percent, but if they do not take part in the reaction or if they do not interfere with the products or the byproducts, then they are not needed to be separated in the reactor feed section or the feed preparation section or in the upstream.

Next question, is the removal of these impurities difficult? So, if there are impurities forms that are say forms azeotrope with the feed or the feed is a gas is I mean the feed is a gaseous system and generally gaseous impure, impurity separation in the gaseous state is not that straightforward and it is expensive then if they do not interfere with the reaction then no need to separate them.

Next question to consider is that these impurities, does these impurities have any tendency or in a chance to poison the catalyst? then it is very important to remove them. The third or the last important criterion to determine to keep it in mind is that whether these impurities take part in any additional side reactions? then also and if these additional side reactions pose a danger to the process or if they are hazardous or toxic, then it is very important to remove them.

The next condition is the addition of feed for stabilizing or enabling products. So, in general this is an important part and we often try to think of that whether this should be considered or not? But please keep it in mind that stabilizing is an important part for our chemical reaction. And in general, these stabilizing chemicals play a big role in the further downstream of the process. So, let us say if the product stream is reactive or is unstable, then does adding any external any additional material helps us to stabilize? even though that creates or that brings in some impurity or addition of trace components, it is still preferable to have that.

So, let us see if a solvent such as water or organic chemical is required for a separation to take place, after the end of the reaction. For example, absorption of a solvent soluble chemical in the gaseous stream then this solvent should be added in the feed to the process, so as to stabilize or enable the product formation in a better way.

The third point is that condition to be kept in mind is that what about the inert feed material, which is necessary to control the exothermic reactions. For example, this catalytic conversion of this partial conversion of propylene to give our acrylic acid, these reaction is generally exothermic. And in this case, we add steam as a thermal ballast. You generally add thermal ballast which will absorb the excess heat and move the reaction mixture out of the flammability limit, and steam as you can see in this reaction does not participate on the reactant side, in fact, it is on the product side effect. So, this is one thing that is generally preferred. Then coming to the case of the inert material. So, often for equilibrium-controlled reaction sometimes it is necessary to add some additional materials so, that we can control the reaction equilibrium in the desired way.

For example, this reaction that you see in your screen, this catalytic dehydrogenation of ethyl benzene, this reaction generally takes place at high temperature around 600 to 750 or 800 degrees centigrade, about at lower pressure less than 1 bar. So, here generally steam is co-fed with ethyl benzene to provide the necessary heat and reduce the partial pressure of ethyl benzene. So, that is what it will prefer. So, this reaction will prefer in the forward direction you try to reduce the pressure of the… this ethyl benzene. So, these are some of the important considerations to be kept in mind for designing a process.

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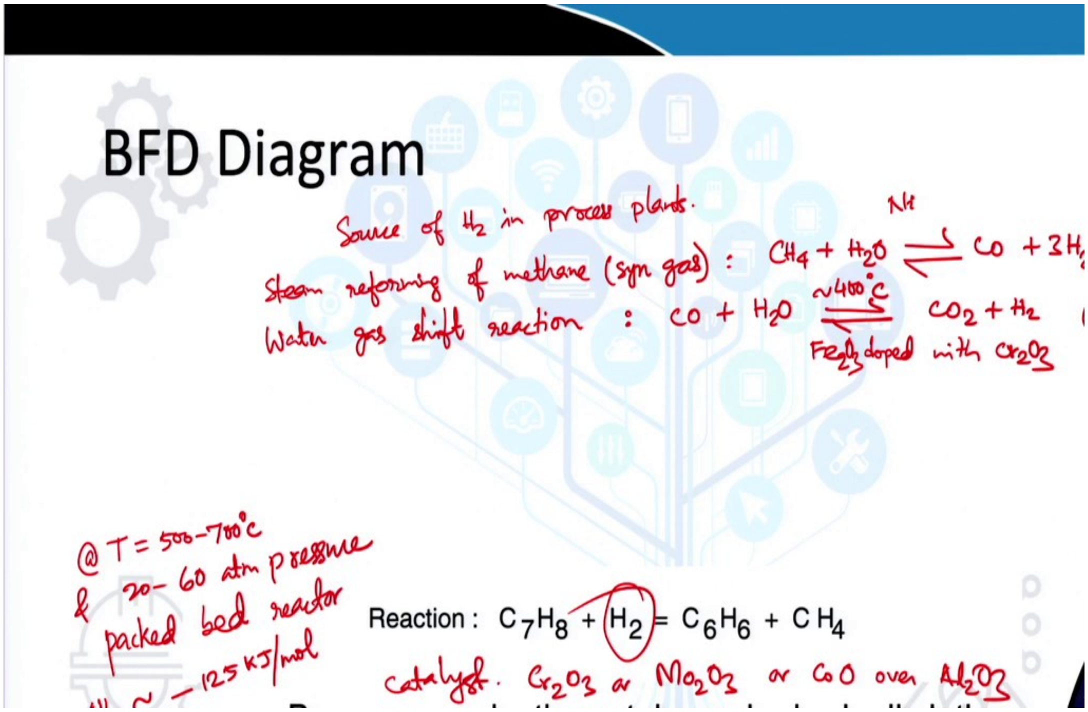

BFD Diagram

Source of H_2 in process plants.

Steam reforming of methane (syn gas) : $CH_4 + H_2O \overset{Ni}{\rightleftharpoons} CO + 3H$

Water gas shift reaction : $CO + H_2O \underset{Fe_2O_3 \text{ doped with } Cr_2O_3}{\overset{\sim 400^\circ C}{\rightleftharpoons}} CO_2 + H_2$

@ $T = 500-700^\circ C$
& 20-60 atm pressure
packed bed reactor
~ -125 kJ/mol

Reaction : $C_7H_8 + H_2 = C_6H_6 + CH_4$

catalyst. Cr_2O_3 or Mo_2O_3 or CoO over Al_2O_3

Now, coming to Block Flow Diagram, let us talk about an example situation where we have benzene production from toluene hydrodealkylation. So, the reaction is given in your screen and I will just try to help you to frame this Block Flow Diagram, how? So, the first thing is to consider the what about the process conditions? So, generally this reaction takes place. So, this process reaction this toluene hydrodealkylation, this reaction takes place generally at a temperature of 500 to 700 degrees centigrade and 20-60 atmospheric of pressure and this is generally in a packed bed reactor you have this reaction.

So, one of the common questions that comes to the mind is that what is the source of this hydrogen? because you see here for this hydrodealkylation you need hydrogen. So in a process plan what is the source? So, the source of hydrogen in process plants is by two ways: one is the steam reforming of methane, which is nothing but the steam gas reaction that (you are) all of you are, I am sure are aware of. So, this is the steam reforming of methane. So, generally this takes place in the presence of nickel catalyst and the delta H of this reaction is around 200 kilojoules per mole.

Other reaction is the water gas shift reaction. There is also another way, and this is generally also quite popular in petroleum and hydrocarbon industries. So, just to wait just a minute this water gets safe reaction the catalyst is iron oxide doped with chromium oxide and this reaction takes place at around 400 degrees.

There is also another resource of the hydrogen in the process plant or in the petroleum and hydrocarbon industry is in catalytic reforming. So, in the process of trying to in the reformer, you will see that due to the dehydrogenation of various petrochemicals, there is enormous production of hydrogen.

So, generally these are the productions of or the source of the hydrogen. So, and what is the source of toluene? So, toluene naturally occurs at very low levels in the crude oil and it is also a byproduct of gasoline reforming, catalytic reforming of gasoline also produces a lot of toluene as a byproduct. So, now this, did I tell you the catalyst for the dehydration? So, the catalyst for this dealkylation is generally chromium oxide or you can have molybdenum oxide or cobalt oxide supported over alumina and this reaction is highly exothermic. So what does this tell you?

From the reaction conditions you understand that you need to have two feed preparation units, because the reaction temperature is very high and then you will have a reactor and (I am) just the simplest case and then you will have this product formation forming benzene and methane. So, you would like to generally benzene will be easily can be brought down to a liquid state. So, you can have a gas-liquid separation and there will be hydrogen and methane in the gas separation units. If you further want to reuse the hydrogen, say you might need a recycled stream isn’t it? for the hydrogen after separation or without separation, depending on what is the presence or how much is the presence of this methane in the system.

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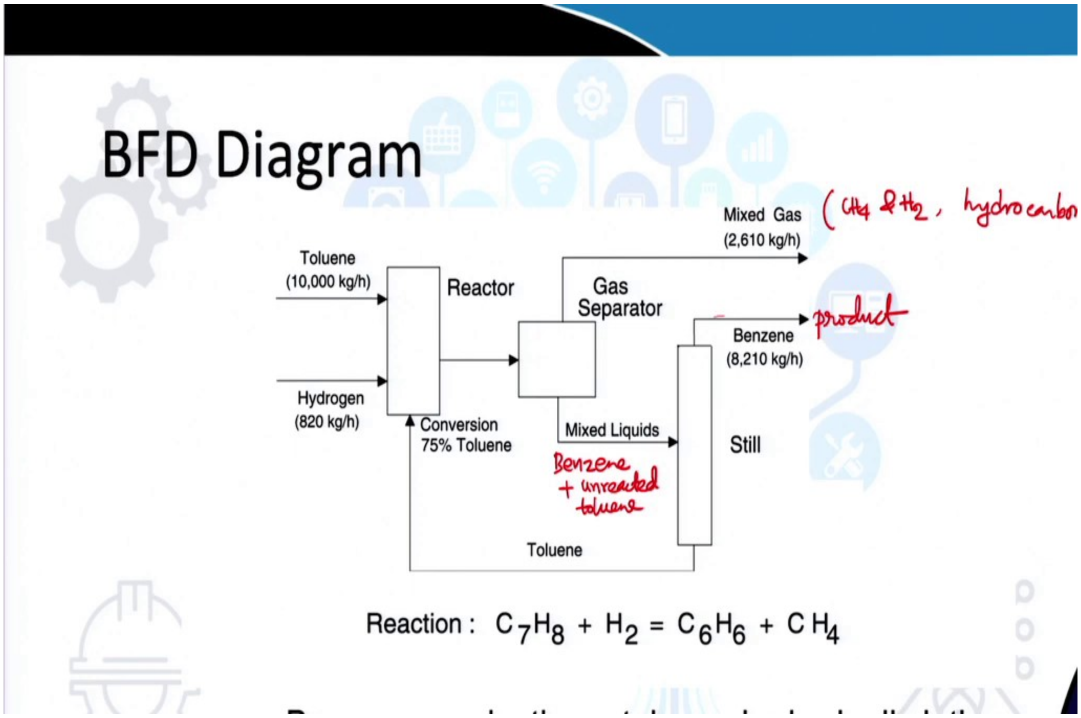

BFD Diagram

Reaction : $C_7H_8 + H_2 = C_6H_6 + CH_4$

So, this is how the system would look like so, you would have a toluene and hydrogen. So, of course, here we are talking about the block flow diagram. So, I have not included the feed preparation unit for toluene hydrogen, because please note that the reaction condition is high temperature and high pressure. So, you cannot use toluene hydrogen just from a storage. This has to be prepared or there has to be some increase or raising their temperature close to the reaction temperature.

So, once the reaction is over then again you need to have a system either to cool it down or to depressurize, so that you have this benzene and the unreacted gas as well as methane. So, what are the unreacted gas? You generally have in this case you will be having methane and sorry, you will be having yes methane and hydrogen as well as there is a possibility of presence of other hydrocarbons. Since it is a hydrocarbon reaction so, you cannot exclude the possibility of the presence of other hydrocarbons. Generally, these are the streams represent along with benzene.

Now, this benzene has to go to a separator because we will be having some unreacted toluene sorry, unreacted toluene in the system. So, this is benzene plus unreacted toluene. So, again the unreacted toluene is sent back to the reactor and benzene is taken out as our desired product. So, this is the very simplest block flow diagram where we haven't included any of the these components for pre-treating the reactor feeds the preparation part or the separator or the this separator feed preparations all these things are not included. So, this is a very basic design or a flow structure of this toluene hydrodealkylation.

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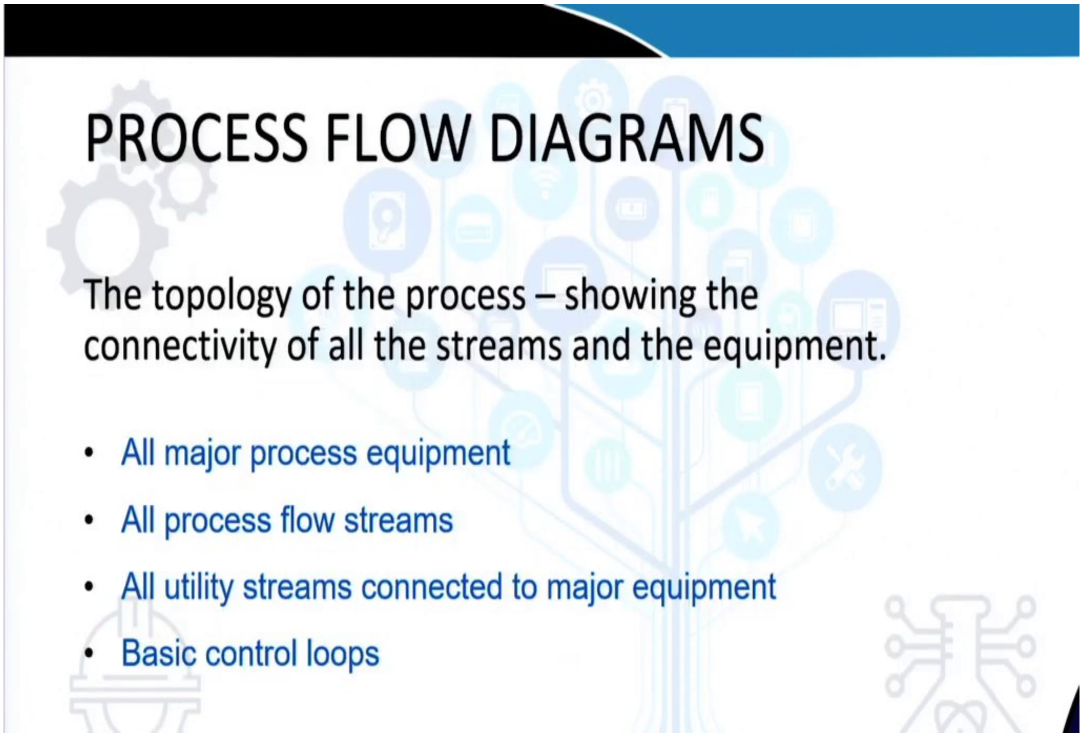

PROCESS FLOW DIAGRAMS

The topology of the process – showing the connectivity of all the streams and the equipment.

- All major process equipment
- All process flow streams
- All utility streams connected to major equipment
- Basic control loops

Next, I am going to talk about the process flow diagrams, and the process flow diagrams are the next level of detail process diagrams, where not only do you show the major equipments and the streams, you also show this control loops and all the blocks or all the units have their own symbols as well as you also try to show that different stream modulation or the stream treatment units or the processes. So, there is a next level of detailing that is present from the block flow diagram. So, that is how you generally synthesize from a block flow diagram to a process flow diagram by adding relevant details.

Now, here let me just enlighten you on some of the guidelines for choosing the separator units. So, generally the separator units are very critical in a process plant, and they generally have or they generally determine most of the cost or economics of the process. So, some of the guidelines comes here is that you should use distillation as the first choice for separation when the purity of the both products are required. Of course, if only distillation is possible there is a significant difference in the relative volatilities. Distillation should be the first choice if purity is concerned.

This is generally the case, and we are not talking about very sophisticated products like for example, pharmaceutical compounds where you need to have extreme high levels of purity for which very fine separation techniques for example chromatography, etc., is required. You can use gas absorption to remove one trace component from a gaseous stream. You can also consider adsorption aD to for removal of trace impurities from gas and liquid streams. You can also consider membranes for gas separation of gases of cryogenic boiling point and relatively low flow rates.

You can consider extraction if you want to purify one liquid from another liquid. Crystallization is to separate two solids as to purify a solid from a liquid stream. You can choose evaporation to concentrate solution of a solid in a liquid. Generally, evaporation comes along with, I mean there is a competition whether to go for evaporation or whether to go for spray drying. But of course, please remember spray drying is not a preferred technique for concentrating a solution. It is generally used (spray drying) to get your final spread product. So, evaporation is actually precedes the spray drying component.

You can use centrifugation to concentrate a solid from a slurry. You can use again filtration to remove solids I mean these are generally quite inevitable choices. The other important part or the important thing is that if your product is of very high value, if a product is a very high value and purity is of extreme concern, as I said before, then go for the sophisticated processes, for example chromatography or you can have very well-defined membrane separation process.

So, for a base case, you must choose a reasonable separation process, but it may be that is that this is not the best choice, but before choosing what is the best choice you are if you are choosing expensive process, it is always advisable to have some basic separation process or treatment processes, so that the load on the sophisticated technique, especially separation technique is reduced. And what is the, there is also a typical guideline for sequencing the separation units. Let me also enlighten you on that. Generally, the largest product stream should be removed fast.

So, what does this mean is that the size of the subsequent separation units are smaller. So, for distillation you should remove the product which has the highest heat of vaporization if possible, as this will reduce the heating and cooling duties of all the subsequent units. Do not in a process, for a good designer, please make sure that you do not recombine or you do not need to recombine the separate stream. So, this may seem quite obvious like but for a big process having multiple streams this may not always or it may be difficult to satisfy. Do the easy separation fast or the low expensive one should be done later you should do the fast easier once.

It is generally not advisable to waste raw materials, but you do not over purify stream based on their uses. Remove the hazardous or the corrosive materials fast because they will corrode or can be hazardous to all the remaining units and as I said use the less expensive or crude separation technique first before going for a sophisticated one. So, you should prefer (let us say) liquid extraction first before moving towards chromatography.

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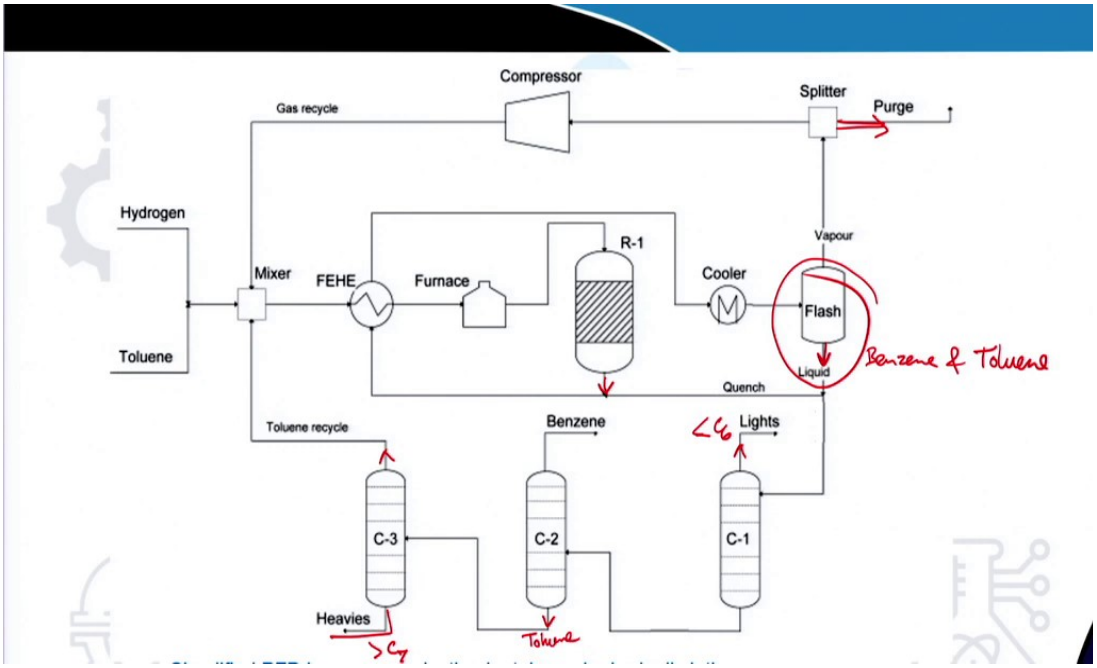

So, having said all this here is a slightly detailed process flow diagram of the toluene hydrodealkylation and you can see that here I have made a reactor feed preparation unit. So, toluene and hydrogen first goes to the fired heat exchanger because since I have set the temperature is if it is more than 150 or 200, you often need a fired heat exchanger or in this case the temperature is close to 500. So, you need also furnace to further heat it up. The furnace is nothing but the heater then it goes to the heater reactor then it again goes and passes. So, you see that the outlet stream of the production of the reactor is actually again exchanged there is a heat exchanger here because there is a lot of heat on the product side which can be used to preheat the reactant. So, you are using the product to preheat your reactant and then it goes to the cooler. So, there is where you will get the liquid benzene, but that is where you get this flash tongue. So, if you further reduce the pressure, you will be getting so, this liquid that is coming down from the flash is mostly benzene and toluene and the top product of the flash are the vapor components – generally hydrogen and methane.

So, there is one part each component is there so, that you can manipulate the amount of methane that is recycled back we do not want to meet him we want hydrogen but then again separating hydrogen methane is very expensive. So, is a technique is to purge or to take out some of the this methane and hydrogen all together.

So, you do not recycle the entire whatever this methane and hydrogen that is (I mean) the hydrogen that is unutilized. So, you remove all your waste some of the or take out some of them product even though that is useful for this case and again it is passed through the compressor as a pretreatment step and again because it went through the flash, So, the pressure is reduced, so you need compression. And then again it is sent back to the mixture for the subsequent processes. For the case of the liquid stream, first it is this, first distillation unit is generally to remove all the lower hydrocarbons less than C6. So, there is a possibility that any hydrocarbon reaction will generally produce a series of hydrocarbon materials. So, in order to have more purity on the products in this case, the first component the first distillation unit is to remove the smaller components or the alkanes or the lower molecular weight compounds or the lower carbon number compounds.

The second one is of course, trying to separate benzene, and the bottom product of the separation of this component is enriched with toluene and heavier hydrocarbon, and since if you are worried about the purity of toluene that is sent back, you can have an additional separating unit., so, that the heavier compounds that is greater than C7 are actually removed and toluene is very nicely purified and sent back to the system.

So, this is a way of, if you think that the purity of the product is very vital, then you should have additional separation units, that is from the cost calculation that needs to be decided or taking a decision on.

So, with this I would like to conclude today in this lecture. Thank you. I hope all of you have liked it.