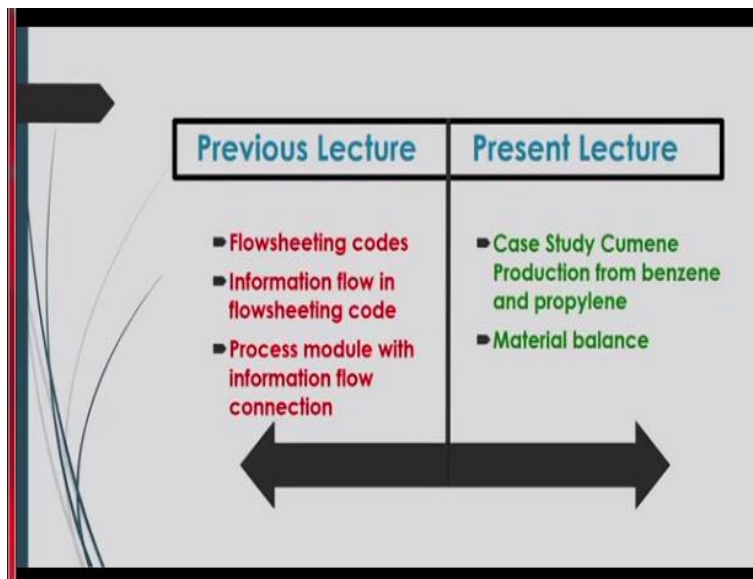


Basic Principles and Calculation in Chemical Engineering
Prof. S. K. Majumder
Department of Chemical Engineering
Indian Institute of Technology-Guwahati

Module-12
Lecture-34
Case Study: Cumene production

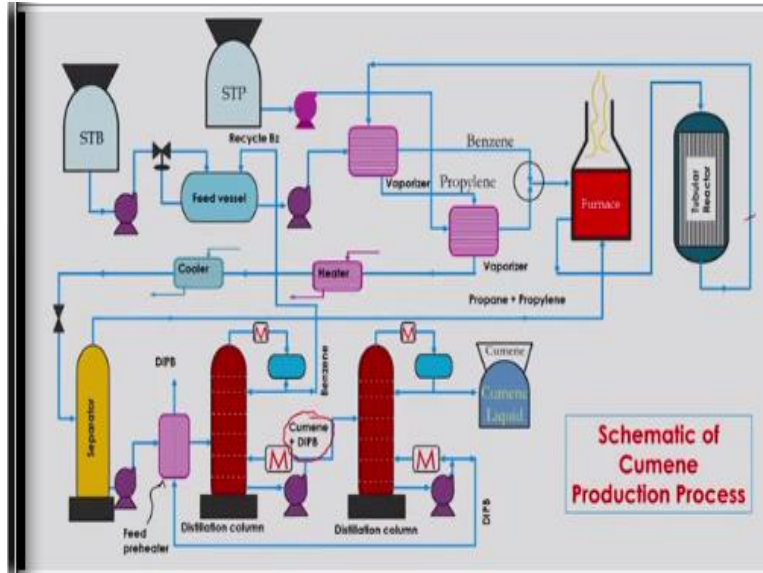
Welcome to massive open online course on basic principles and calculations and chemical engineering. So we will describe here a case study for a process under module 12 and in this module will describe a case study of Cumene production from you know benzene and propylene. And we will focus on only material balance of this you know this Cumene production process.

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And in the successive lecture we will try to describe about to that energy balance equation and it is solution. And in the previous lecture, we have described the flowsheeting codes information flow in flowsheeting codes process module with information flow connection like this. So, here is we will describe about that cumene production from benzene and propylene as a case study with whatever we have learned earlier.

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Material balance and energy balance and other you know solution method of those process, even also how to solve that material and energy balance whether it is linear or nonlinear equations. And also what are the different codes are there that we have learned. Now let us consider here on schematic of this cumene production process, see here this cumene is produced from the reaction of benzene and propylene.

There are several units are actually being used for this particular cumene production industrially. Here the complete you know process diagram or you can say schematic diagram of the processes given. Now the main process unit for this cumene production which are used or like you know that vaporizer, reactor, separator and distillation column. Other small you have process units also are required and you know accessory of those you know equipment, many equipments there.

So let us describe first this you know cumene production process here. You will see that in this flow diagram here you will see that on STB and here STP, STB is basically the storage tank for benzene and STP is the storage tank of propylene. Now these benzene and propylene from this storage tank is you know send to you know a furnace to raise it is temperature for the reaction in a tubular reactor here.

Now it will be sent through vaporizer, benzene will be passing through the benzene vaporizer and propylene will be send to the propylene vaporizer. And then these 2 streams should be mixed

in a you know mixer and then it will be send to a you know furnace to raise it is temperature. Now you will see that whenever you will be sending or as per process you know industrially that benzene .

The fresh benzene from this storage tank it will be mixed with some recycled benzene which is basically coming from distillation where this cumene and also it is byproducts along with the benzene is separated. And after separation the benzene components will be you know recycle to this, you know fresh this benzene. And then mixer of this fresh benzene and recycle benzene it will be you know send through it is vaporizer.

And then it will be mixed with that propylene and then it will be going through that furnace. After furnace you know that it will go through the reactor where this benzene and propylene will be reacting at a certain temperature and pressure in this reactor. And after reaction you will see some products will be coming out like you know that cumene, you know di isobutyl, you know isopropyl benzene.

And also you will see that unreacted benzene unreacted propylene will be you know coming out from that reactor as a you know outlet stream. And then it will be passed through the you know benzene vaporizer where this you know heated up of this product will be used to you know raise the temperature of that you know benzene feed by this vaporizer using these outlet streams of reactor.

And then it will be you know again sent through that propylene vaporizer, where this you know temperature will be you know or heat will be used to vaporize this propylene at a certain temperature. After that it will be again heating and then cooling and then you know it will be sent to a separator. And in the separator you will see that unreacted propylene and propane where propane is actually basically coming with that propylene.

Because propylene is not 100% pure some fractions of that propane will be there along with that propylene. So those propane and then propylene will be separated by the separator and from the top part this you know this propane and propylene it will be used for heating up that you know

mixer of benzene and propylene in a furnace. And from the separator you know other part of this product like.

You know that benzene unreacted benzene and cumene and byproduct di isopropyl benzene isopropyl you know butane . It will be you know that separated in the distillation column. So this distillation column can be named as benzene distillation column because here the benzene will be you know separated out from that benzene column and it will be recycled to you know mix with that you know fresh benzene.

And from this benzene distillation column this cumene and DIPB, it will be sent to you know that again another distillation column this distillation column is called cumene distillation column where this mixer of cumene and you know DIPB will be separated. And in the over heat product that cumene will be separated, there will be certain percentage of cumene of product as per that you know requirement of that you know process.

And from the bottom part of that cumene distillation column, this DIPB will be you know taken out and it will be used for you know preheating that output of that separator of that cumene and DIPB mixer. And then DIPB would be you know taken out as a product there. Now in this whole process we are seeing that several you know process units are required and in each process units you will see that there will be some inputs and outputs.

And some also units will have that recycle stream along with the fresh stream and then after that mixing up that recycle stream and it will be sent to another stream and it will mixed and then process further. So this is your whole process actually for the production of cumene. Now in this case you will see that there will be a certain reaction will be going on for the production of this Cumene.

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Background

- Raw material propylene and benzene are used for the production of cumene.
- Main Reaction:

$$\text{C}_3\text{H}_6 + \text{C}_6\text{H}_6 \rightarrow \text{C}_9\text{H}_{10}$$

Propylene
Benzene
Cumene
- By-Product Reaction:

$$\text{C}_3\text{H}_6 + \text{C}_9\text{H}_{10} \rightarrow \text{C}_{12}\text{H}_{18}$$

Propylene
Cumene
Di-isopropylbenzene(DIPB)

These reactions can occur in liquid and gas phases, but high conversion is obtained at gas phase reactions, the catalyst like solid phosphoric acid are replaced by zeolites and the catalytic conversion reaction are held in shell and tube reactors rather than packed fixed bed reactors.

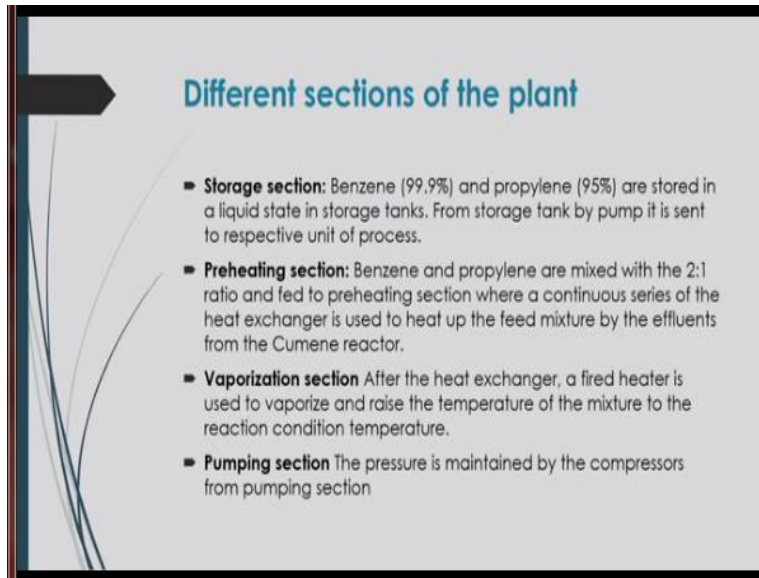
The raw material basically the propylene and you know benzene, main reaction here it is given like propylene will be reacting with that benzene and it will be produced there you know cumene. And as a byproduct there again that produced cumene along with that you know propylene there will be a reaction and then byproduct like isopropyl benzene will be you know produced. Now, these reactions can occur in liquid and gas phases here.

But high conversion is obtained at the gas phase reactions, the catalyst like solid phosphoric acid are actually replaced by zeolites and catalytic conversion reactions are held in shell and tube reactor rather than packed bed fixed reactors. Now this is interesting that for this reaction, you are using that solid phosphoric acid instead of zeolites. Because of that you know increasing the efficiency of that reaction and there will be some catalytic conversion reaction here in this reactor.

Now there are several different type of reactors are there but generally you know packed bed reactors are being used for this type of reactor to get the contact between gas and liquid. But here since there will be sorted temperature to be maintained there. So it is better to use that shell and tube reactors there where in a tube side that mixture of you know that benzene and toluene will be benzene and propylene will be you know passed through that reactor in presence of phosphoric acid catalyst.

Whereas in the shell sides there may be you know streams will be supplied for changing the R you know that controlling that temperature there.

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So this is the background here, now different sections of the plant or like you know storage section, preheating section, vaporization section, pumping sections there. In the storage section you will see that benzene it will be 99.9% purity and propylene it is 95% purity whereas remaining 5% maybe mixed with propane are stored in a liquid state in a storage tanks. Now from storage tanks by pump it is sent to respective unit of processes.

Preheating section where benzene and propylene are mixed with the you know 2 : 1 ratio and it these are fed to preheating section where a continuous series of heat exchanger is used to heat up the feed mixer by the effluents from the cumene reactor. And the vaporization section after the heat exchanger, a fired heater is used to vaporize and raise the temperature of the mixer to the reaction condition temperature.

And in the pumping section, the pressure is maintained by the compressor from the pumping section. So that at a certain pressure that liquid mixer or gaseous mixers to be sent to the process unit.

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Different sections of the plant

- Storage section:** Benzene (99.9%) and propylene (95%) are stored in a liquid state in storage tanks. From storage tank by pump it is sent to respective unit of process.
- Preheating section:** Benzene and propylene are mixed with the 2:1 ratio and fed to preheating section where a continuous series of the heat exchanger is used to heat up the feed mixture by the effluents from the Cumene reactor.
- Vaporization section** After the heat exchanger, a fired heater is used to vaporize and raise the temperature of the mixture to the reaction condition temperature.
- Pumping section** The pressure is maintained by the compressors from pumping section

In the reactor section you will see that a tubular reactor is used to withstand the pressure to 25 atmosphere and 350 degree Celsius. The reactor tubes are filled with catalyst and the feed is charged from the top. The feed gas reacts and pass over the catalyst bed with 99% conversion of propylene and outlet stream is sent to the recycle and purification section. However they are you know different type of separators or distillation columns are used.

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Different sections of the plant (contd..)

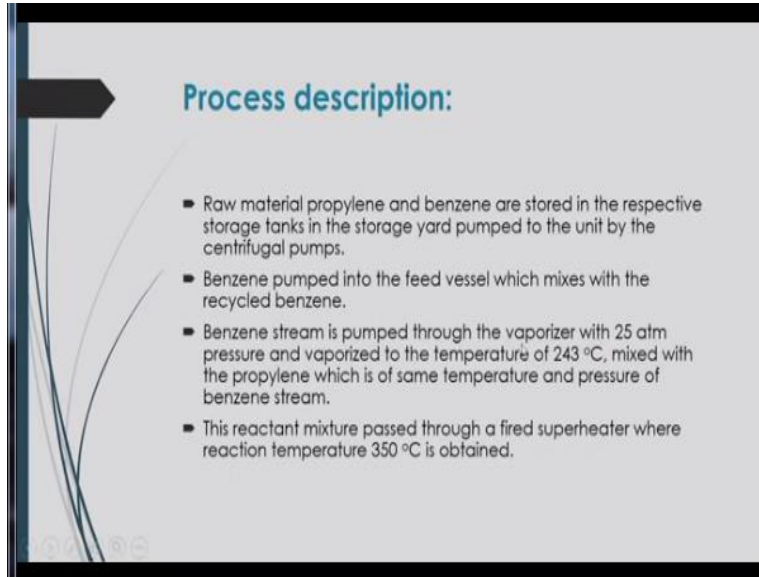
Separation and purification section:

- Unreacted benzene is separated in a distillation column from the effluent obtained from the reactor and the recovered benzene is recycled to the feed stream,
- As per side reaction by-product (di- isopropylbenzene (DIPB)) is generated which is separated by distillation from the product mixture
- The by product di- isopropylbenzene is separated in a sieve tray distillation column which is of 99 percent pure.

Now in that separation and purification section unreacted benzene which is separated in a distillation column from the effluent obtained from the reactor. And the recovered benzene by the distillation process in the separator is recycle to the feed stream. As per you know side reaction, there will be a byproduct this called di isopropylbenzene which will be produced as a

byproduct and it is generated. And then it is separated by distillation from the product mixer. The byproduct that di isopropylbenzene is separated in a sieve tray distillation column which is of 99% pure.

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Process description:

- Raw material propylene and benzene are stored in the respective storage tanks in the storage yard pumped to the unit by the centrifugal pumps.
- Benzene pumped into the feed vessel which mixes with the recycled benzene.
- Benzene stream is pumped through the vaporizer with 25 atm pressure and vaporized to the temperature of 243 °C, mixed with the propylene which is of same temperature and pressure of benzene stream.
- This reactant mixture passed through a fired superheater where reaction temperature 350 °C is obtained.

Now what is the process description for that you have to first of all know that how this process is going on. In this case raw material propylene and benzene are stored in the respective storage tanks. In the storage yard and then pump to the unit by the centrifugal pumps, benzene pumped into the feed vessel which mixes with the recycled benzene. And benzene stream is pumped through the vaporizer with 25 atmospheric pressure and vaporized to the temperature of 243 degrees Celsius.

And then mixed with the propylene which is of same temperature and pressure of benzene stream. Now this reactant mixer passed through a fired super heater where reaction temperature 350 degrees Celsius is to be obtained.

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Process description (contd..)

- The vapour mixture is sent to the reactor tube side which is packed with the solid phosphoric acid catalyst supported on the kieselguhr
- The exothermal heat is removed by the pressurized water which is used for steam production
- The effluent from the reactor i.e., cumene, p-DIPB, unreacted benzene, propylene and propane with temperature 350 °C is used as the heating media in the vaporizer which is used for the benzene vaporizing

Now the vapor mixer is then sent to the reactor tube side which is packed to the solid phosphoric acid catalyst supported on the kieselguhr. The exothermal heat is there recovered by the pressurized water which is used for stream production and it is passed through the shell side of that reactor. The effluent from the reactor that is cumene and byproduct p-DIPB, unreacted benzene, propyl and propane which are not taking part in the reactor for reaction with temperature 350 degrees Celsius is used as the heating media in the vaporizer which is used for the benzene vaporizing.

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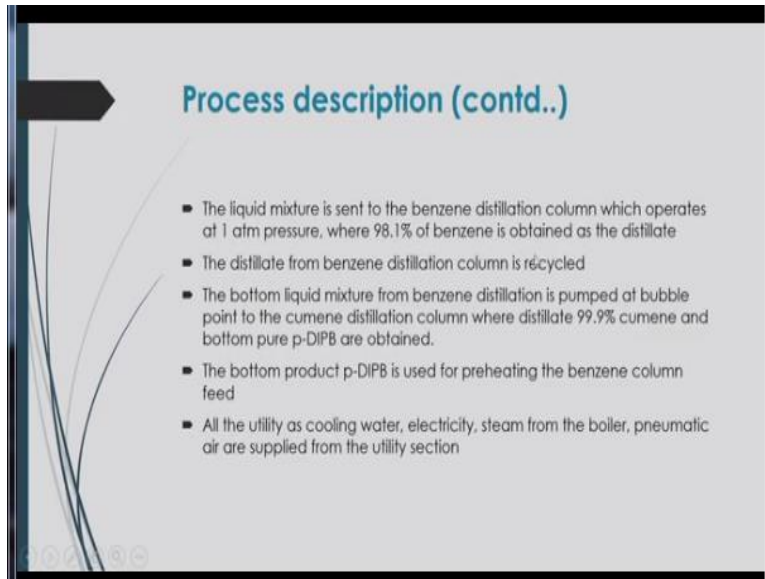
Process description (contd..)

- After that the effluent is cooled to 40 °C in a water cooler
- Propylene and propane are separated from the liquid mixture of cumene, p-DIPB, benzene in a separator operating slightly above atm
- The pressure is controlled by the vapour control valve of the separator,
- The separated fuel gas (propylene & propane) is used as fuel for the furnace.

After that the effluent is cooled to 40 degrees Celsius in a water cooler, propylene and propane are separated from the liquid mixer of the cumene DIPB, benzene in a separator that is operated

slightly above atmospheric pressure. The pressure is controlled there by the vapor controlled valve of the separator. The separated fuel gas that is a mixture of propylene that is unreacted and propane is used as a fuel for the furnace.

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Process description (contd..)

- The liquid mixture is sent to the benzene distillation column which operates at 1 atm pressure, where 98.1% of benzene is obtained as the distillate
- The distillate from benzene distillation column is recycled
- The bottom liquid mixture from benzene distillation is pumped at bubble point to the cumene distillation column where distillate 99.9% cumene and bottom pure p-DIPB are obtained.
- The bottom product p-DIPB is used for preheating the benzene column feed
- All the utility as cooling water, electricity, steam from the boiler, pneumatic air are supplied from the utility section

However the mixture of propylene and benzene to be you know fired or vaporized to a temperature of 350 degree Celsius. Then the liquid mixer is sent to the benzene distillation column which operates that 1 atmospheric pressure where 98.1% of the benzene is obtained as the distillate. And this distillate from the benzene distillation column is then recycled and it is mixed with the fresh benzene.

The bottom liquid mixer from the benzene distillation is then pumped at bubble point to the Cumene distillation column. However distillate will have 99.9% cumene and bottom products will have pure you know para di isopropyl benzene. And then bottom product of this p-DIPB is used for pre-heating the benzene distillation column. For each preheating of heat all the utility they are water being used like cooling water, electricity stream from the boiler, pneumatic air are supplied from the utility section.

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Overall material balance

- All material balance calculations are based on the principle of conservation of mass, which states that matter can neither be created nor be destroyed, but they may undergo physical or chemical changes.
- Rate of mass input = Rate of mass output + Rate of mass accumulation
- For steady state operation where accumulation is constant,
- Rate of mass input = Rate of mass output
- The material can refer to a balance on a system for
- Total mass; Total moles; Mass of chemical compound; Moles of the chemical compound; Moles of an atomic species; Volume

Now then you have to do the overall material balance for this whole process there. Now all material balance calculations, whatever we have described earlier, what is the principles that same principles to be used here. And those material balance calculations will be based on the principles of conservation of mass which states that matter can neither be created nor be destroyed but they may undergo physical or chemical changes.

In that case, according to that material balance equation, we can say that rate of mass input that will be equals to rate of mass output + rate of mass accumulation. For steady state operation where accumulation is constant, the rate of mass input that will be equals to rate of mass output. The material can refer to a balance on a system for total mass, total moles, mass of chemical compounds, moles of the chemical compound or mass of an atomic species and also volumes.

So based on this you can do the overall material balance. Now in this case, for the whole process, you will see there will be a some data assumption. Our main objective is to produce 500 tons per day of cumene production this is our goal.

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Data Assumption

Objective	500 tons /day of Cumene production
Conversion of propylene	99%
Product molar selectivity cumene to p-DIPB is	31:1
Propylene purity in feed is	95%
Propane in feed	5%
Benzene purity in feed is about	> 99.9%
Molar feed ratio of benzene to propylene	2:1
Top product of benzene column is	98.1% benzene and 1.9% cumene
Top product of cumene separation column is	99.9 mole % cumene 0.1% p-DIPB
Bottom product of cumene separation column is	100 mole % p-DIPB
The propane is assumed as a tie substance which does not participate in the reaction, it is used as fuel.	

So in that case as per reaction, it is seen that there will be a 99% propylene conversion and product molar selectivity of cumene to para di isopropyl benzene is 31 : 1. And propylene purity in the feed is 95% remaining is propane, benzene purity in the feed is about 99.9% remaining maybe other components there. Like you know whatever benzene streams is coming as a recycle they are some small amount of cumene maybe will be mixed with that.

So that cumene will be there in the benzene streams, molar feed ratio benzene to propylene it will be 2 : 1 top product of benzene column will be 98.1% benzene and 1.9% of cumene. Top product of cumene separation column there will be 99.9 mole percent of cumene whereas remaining will be byproduct, bottom product of cumene separation column it will be 100% you know byproduct it is assumed.

And the propane whatever is assumed as a tie substance here as a you know in our material which is not taking part in the reaction does not participate in the reaction and it is generally being used as a fuel for the furnace.

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Basis

- 500 tons /day of 99.9% CUMENE PRODUCTION
- 500 tons/24 per hr of pure cumene = $(500 \times 1000) / (24 \times 120.19) \times 0.999 = 173.16$ kmole/hr of pure cumene
- Primary reaction:**
 $\text{CH}_2\text{-CH}_2\text{-CH}_2$ (propylene) + C_6H_6 (benzene) \rightarrow C_9H_{10} (cumene)
- Side reaction:**
 $\text{CH}_2\text{-CH}_2\text{-CH}_2$ (propylene) + C_9H_{10} (cumene) \rightarrow $\text{C}_{12}\text{H}_{18}$ (DIPB)

As per reaction 1 mole of DIPB production 2 moles of Propylene required

So in this case, basis is that you have to produce 99.9% pure cumene at a rate of 500 tons per day. Now as per calculation you can say that 500 tons per day means 500 tons divided by 24 hours of day. So it will be coming as here 500 into 1000s that is kg divided by 24 into you know 120.19 it will be converting that is 24 hours in a day and into 120.19. This is basically the molecular weight of you know cumene.

So you can get in terms of unit of kilo moles per hour, but since you have to produce 99.9%. So actually this as per calculation 173.16 kilo mole per hour of pure cumene is to be used for reaction, what is the primary reaction that already we have described in our previous slides there will be propylene that will reacting with benzene and it will give you the cumene as per this reaction.

And parallely there will be a side reaction like this propylene again with produced cumene would be reacted and it will give you that, you know byproduct of the DIPB. In that case as per reaction 1 mole of the DIPB will be produced based on 2 moles of propylene used for the reaction.

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Propylene used for the cumene and DIPB:

- So for cumene, propylene required is 173.16 kmole/hr

$$\text{Selectivity} = \frac{\text{mole of cumene produced}}{\text{mole of DIPB produced}} = \frac{31}{1}$$

- Conversion of propylene is 99%
- Let x kmole of DIPB is formed, then, cumene formed is 31x
- Implies, $31x = 173.16$ or $x = 5.59$
- DIPB formed is = 5.59 kmole/hr

Now propylene used for the Cumene and DIPB as per that you know assumption of that selectivity. We can say that the propylene required is 173.16 kilo mole per hour, for that target amount of Cumene production. And as per selectivity it is given the 31 : 1, we can say that conversion of propylene if it is 99% then what should be the amount of DIPB to be produced based on that you know reaction.

Let x kilo mole of DIPB is formed then cumene formed will be as 31 into x as per selectivity, whose implies that 31 x will be equal to 173.16, that means x will be is equal to after calculation 5.59. So the amount of DIPB formed is simply 5.59 kilo mole per hour.

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PROPYLENE BALANCE	
Propylene required for cumene	= 173.16
Propylene required for DIPB	$2 \times 5.59 = 11.17$
Total propylene required	= 184.34
Propylene conversion = 99%	
So, Propylene in Feed	$184.34/0.99 = 186.20$
Unreacted propylene =	$186.20 - 184.34 = 1.86$

PROPANE PRESENT:	
As Propylene feed is 95% pure and rest of propane	
Total propylene feed (pure propylene + propane) is	$= 186.20/0.95 = 196.0$ kmole
Propane in feed	$= 196.00 - 186.20 = 9.80$ kmole

And then you have to do that propylene balance, now propylene required for cumene is as per you know reaction stoichiometric is 173.16, propylene required for DIPB this is 2 times of that, it will be is equal to 5.59 into 2 that will be 11.17. Now total propylene then required if you sum it up, you will get it to 184.34 because this propylene give you the cumene and also DIPB. So total amount will be required this 184.34 kilo mole.

Now since the propylene conversion is 99%, we can say that the propylene in feed will be this amount, you have to divide this you know 184.34 which is taking part for reactions divided by it is purity that is 99%. So if you divide it you will get that what will be the propylene in feed was there. And then unreacted propylene will be there if you subtract this you know 186.20 and 184.34 then you can get what would be the unreactive propylene.

So this is basically 1.86 kilo mole, now as per propylene feed since it is 95% pure and rest of propane, you can see that total propylene feed that is pure propylene + propane that will be is equal to to here 186.20 divided by 0.95 it will give you 196.0 kilo mole. Then remaining amount will be you know that propane which will be you know calculated as this is your total amount of propylene pure + propane.

If you subtract this 186.20 which is a fed there for this propylene if you subtract it then you will get the remaining amount of 9.80 as a propane.

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BENZENE BALANCE		
Benzene required for cumene	173.16	✓
Benzene required for DIPB	5.59	✓
Total benzene required	178.75	✓
Given: Benzene to propylene feed ratio =	2:1	✓
So, benzene to be feed (total Propylene require x 2)	$184.34 \times 2 =$	368.37 ✓
Unreacted benzene	$= 368.37 - 178.75$	189.92 ✓

Feed vessel:	
Fresh feed of benzene	$= 178.75$ Kmole ✓
Recycle feed of benzene along with cumene (1.19% of recycle = 3.68 kmole) ✓	$= (189.92 + 3.68) = 193.60$ Kmole } ✓
Mixed feed of benzene	$= 178.75 + 193.60 = 372.35$ kmole ✓

Then you have to do the benzene balance, benzene required for the cumene as per reaction it is 173.16 kilo mole. Benzene required for DIPB it is 5.59 total benzene then required if you sum it up you will get and it is given that benzene to propylene feed ratio should be 2 : 1. So you can say that benzene to be feed total propylene required into 2 that will be to is equal to here 368.37 kilo mole.

Now, unreacted benzene will be then remaining whatever you know there after you know useful for the reaction, now it will be here 189.92. Then you have to do the material balance for the individual unit like feed vessel here one important unit. So in the feed vessel there you will see that fresh feed of benzene is coming in and recycle feed of benzene along with cumene that is 1.19% of recycle that will be 3.68 kilo mole as per calculation.

So total amount of benzene feed is 178.75 plus here recycle amount 3.68, so it will be coming as here, you know that 193. you know 60. And you know that mixed feed of benzene that will be is equal to $178.75 + 193.60$ that will be you know that 372.35.

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Balance around reactor	
Feed = mixed feed of benzene (benzene + cumene) + Feed from STP (pure propylene + propane feed)	= $372.35 + 196.00 = 568.35$ kmole
Output of reactor = Input + Generation - Consumption ✓	= $1.86 + 189.92 + 176.84 + 5.59 + 9.80 = 384.01$ kmole
For propylene: Output = $186.20 + 0 - 184.34 = 1.86$ ✓	
For benzene: Output = $368.67 + 0 - 178.75 = 189.92$ ✓	
For cumene: Output = $3.68 + 173.16 - 0 = 176.84$ ✓	
For DIPB: Output = $0 + 5.59 - 0 = 5.59$ ✓	
Propane: output = $9.80 + 0 - 0 = 9.80$ ✓	

Now balance around the reactor, in the reactor feed will be mixed feed of benzene + feed from STP. That mixed feed of benzene, it is generally that is 372.35 as per calculation here in the slides. And then you have to add that what is coming from the you know STP that is propylene storage tank, so this total moles of this you know feed will be as per reactor. Now from the you know reactor after reactions, what will be the you know output stream, what will be the amount of that.

Now output of the reactor can be calculated based on that, you know material balance, in that case you have to consider that generation and consumption since in the reactor there will be a reaction. Now as per that, you know material balance equation, we can write output of reactor will be is equal to input + generation – consumption. So for that, if we considered that only propylene here, so for propylene output will be is equal to $186.20 + 0$.

Here there is no generation of this propylene and then consumption will be 184.34 that will come 1.86. Now the for benzene similarly you can do it will be as 189.92, for cumene it will be 176.84, in the same fashion if you do the balance for DIPB it will be as 5.59. And for propane since there is no reaction or consumption or generation there. We can say that for DIPB and propane output will be like this, so what will be the total amount of output of that reactor.

If you sum it up all those components of this propylene output, benzene output, cumene output, DIPB output and propane output you can get this 384.01 kilo mole.

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Balance around separator	
Input = Output of reactor	= 384.01 kmole ✓
Top = unreacted propylene + propane	= <u>1.86</u> + <u>9.80</u> = <u>11.66</u> kmole
Bottom (output of separator other than propylene and propane)	<u>384.01</u> - <u>11.66</u> = <u>372.35</u> kmole

After that you have to do the balance around you know separator. Now in the separator what will be the input and output of the reactor. So you will see that whatever you know input of the separator that of course will be output of the reactive. Because same amount of reactor as a output it will be coming to that separator as an input. So it is 384.01 and in the top of this you know separator it will come as unreacted propylene and propane compound.

So, it will be $1.86 + 9.80$ total amount will be 11.66 kilo mole and in the bottom there will be output of separator other than propylene and propane. So that separator output as a propylene and propane amount other than that is you know propylene and propane amount will be then $384.01 - 11.86$. You have to subtract that, you know propylene and propane amount there, then you can get 372, your 35 kilo mole for this, you know separator from the bottom.

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Balance around Benzene distillation column

Input (bottom of the separator) = 372.35 ✓

Give: Top product contains 98.1 mole % benzene; assume all benzene is collected in top only then;

Benzene balance:
 $189.92 \text{ (unreacted)} = D \times 0.981$ ✓

Top product (D) = 193.60 kmole

Cumene present in top product = $193.60 \times 0.019 = 3.68 \text{ kmole}$

Bottom = feed - top
 $= 372.35 - 193.60 = 178.75 \text{ kmole}$

Then you have to do the balance around benzene distillation column. Now in that case, input of this benzene distillation column will be the output of the bottom of the separator. So, as per that it will be 372.35 kilo mole. Now in this case it is given that top product will be containing 98.1 mole percent of benzene. And in that case all the benzene is to be collected in the top and it will be sent as a recycle to the fresh feed.

Now, as per that material balance if you do the benzene balance here, then 189.92 which is unreacted in the reactor, it will be basically the same amount for the distillate of that benzene distillation column. So according to that, we can write this balance equation here, where D is called distillate that is called top product of that benzene distillation column and after calculation it is coming as 193.60 kilo mole.

And then what will be the amount of cumene present in the top product as per that condition, since there 98.1 mole percent of benzene will be there in the you know top product, remaining amount of course will be the cumene. So that cumene can be you know calculated as here 193.60 into 0.019 that will come 3.68 kilo mole. So, this amount of cumene will be along with that benzene and it will be going to that you know vessel where fresh benzene will be mixed with this you know stream of this benzene and cumene product from this benzene distillation product column.

And what will be the bottom product of that benzene distillation column it can be obtained just subtracting that top product from the feed then it will be coming as 178.75 kilo mole.

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Balance around Cumene distillation column

Feed = 178.75 kmole (173.16 (cumene) + 5.59 (DIPB))

Given: top product contain 99.9 mole% cumene
and 100 mole % p-DIPB in bottom.

Cumene balance: ✓

173.16 = Distillate ✓

Top product = 173.16 kmole

Bottom product = feed - top
= 178.75 - 173.16 = 5.59 kmole

After that, you have to do the balance around cumene distillation column, in that case the feed will be 178.75 kilo mole and this is basically what will be the cumene produced as per reaction that is 173.16 + what will to be the byproduct there that is 5.59. So this total amount of this cumene and di isopropyl benzene. It will be you know going into the Cumene distribution column as a feed.

Now since your product will be of 99.9% cumene whereas remaining amount will be as you know that DIPB from the top and from the bottom 100% of that DIPB will be there. So as per that balance equation, if we consider cumene balance, then you can simply write this 173.16 will be as distillate as a top product. So you can write here top product will be 173.16 kilo mole and bottom product will be basically it will be you know that 100% of p-DIPB.

That can be obtained by subtracting that top product from the feed of that cumene distillation column and it will be coming as 5.59 kilo mole.

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Overall plant material balance:

	molwt	INPUT		OUTPUT	
		kmol/h	kg/h	kmole/h	kg/h
BENZENE	78	178.75	13942.44	0.00	0.00
PROPYLENE	42	186.20	7820.28	1.86	78.20
PROPANE	44	9.80	431.19	9.80	431.19
CUMENE	120	0.00	0.00	173.16	20779.60
DIPB	162	0.00	0.00	5.59	904.92
TOTAL		374.75	22193.91	190.41	22193.91

This you know DIPB will be sent to preheat the output of that you know separator to you know send it to the benzene distillation column. Now overall plant then material balance, we can summarize as what will be the input and what would be the output. Now for benzene, what will be the input it is 178.75 kilo mole and output is here 0, whereas propylene there is input is 186.20, output will be here 1.86 kilo mole.

Propane it will be 9.80 output is again same amount and cumene in the input there will be no cumene, here as output whatever target we are fixing that amount that is 173.16 kilo mole will be produced per hour. You can make it in you know mass flow rate also in kg per hour just by multiplying this molar flow rate by their molecular weight respectively. So according to that we can get this total kilo mole per hour for the input is 374.75.

Whereas output it will be total 190.41 kilo mole per hour and as a mass you can say that will be 22,193.91 kg per second and then output will be here the same amount.

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Yield:

As 1 mole of cumene is produced from 1 mole of propylene the Stoichiometry factor is 1

Moles of cumene produced = 173.16 kmole ✓

Moles of reactant fed = 184.34 kmole ✓

The yield of cumene based on propylene: ✓

$$\text{Yield} = \frac{(\text{moles of product produced})(\text{Stoichiometry factor})}{\text{moles of reactant fed to the process}}$$

$$= \frac{(104.16)(1)}{110.88} = 93.93\%$$

Now, if you consider that what will be the yield of that process, as 1 mole of cumene is produced from 1 mole of propylene, the stoichiometric factor is here 1. So moles of cumene produced here 173.16 kilo mole, moles of reactant feed here 184.34 kilo mole. So the yield of the cumene based on propylene, we can calculate here based on the definition of this yield here, moles of product produced into stoichiometric factor divided by moles of reactant fed to the process. So after substitution, we can after calculation as 93.93% yield of the process.

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Equipment wise Material Balance for Cumene Production from Benzene and Propylene

Equipment	Benzene feed pump			Propylene feed pump		Benzene distillation column		Benzene feed	
	Benzene fresh feed			Propylene -propane		Recycle benzene		Benzene mixed feed	
	Mw	kmole	kg	kmole	kg	kmole	kg	kmole	kg
BENZENE	78.00	178.75	13942.44			189.92	14813.84	368.67	28756.28
PROPYLENE	42.00	0.00	0.00	186.20	7820.28	0.00	0.00	0.00	0.00
PROPANE	44.00	0.00	0.00	9.80	431.19	0.00	0.00	0.00	0.00
CUMENE	120.00	0.00	0.00	0.00	0.00	3.68	441.41	3.68	441.41
DIPB	162.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TOTAL		178.75	13942.44	196.00	8251.47	193.60	15255.25	372.35	29197.69

Now we can you know summarize all this material balance equipment wise, there are several equipments that we have seen here for the production of this cumene. Now if we summarize this you know this material balance and it is the amount as per that equipment. We have already

described, but still we can summarize here as like this, what would be the kg or mass fraction or what would be the mass flow rate or you know more mole molar flow rate like this we can you know represent here in this figure.

Now if we consider that benzene feed pump and benzene fresh feed propylene feed pump benzene distillation column and there then in phenyl benzene feed also feed vessel what should be that you know balance equation balance amount there for the benzene, propylene, propane, Cumene, DIPB and then total amount we can get this here. So if we consider the benzene feed pump there benzene fresh feed it will be 178.75 that means 13942.44 for benzene.

Similarly for here propylene what will be the amount, propane what will be the amount and cumene DIPB and total what will be that. And similarly you can summarize it based on that you know propylene feed pump, what will be the you know amount of propylene propane mixer and what will be that input and output for respective you know compound that you can get from this table, it is given here.

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Equipment wise Material Balance for Cumene Production from Benzene and Propylene

Equipment	Reactor		Reactor		Flash drum (separator) top		Flash drum (separator) bottom		
	Reactor input		Reactor output		Fuel gas		Feed to the benzene column		
	Mw	kmole	kg	kmole	kg	kmole	kg	kmole	kg
BENZENE	78.00	368.67	28756.28	189.92	14813.84	0.00	0.00	189.92	14813.84
PROPYLENE	42.00	186.20	7820.28	1.86	78.20	1.86	78.20		0.00
PROPANE	44.00	9.80	431.19	9.80	431.19	9.80	431.19		0.00
CUMENE	120.00	3.68	441.41	176.84	21221.01	0.00	0.00	176.84	21221.01
DIPB	162.00	0.00	0.00	5.59	904.92	0.00	0.00	5.59	904.92
TOTAL			37449.16	384.01	37449.16	11.66	509.40	372.35	36939.77

Similarly for reactor input reactor output flash drum that is separator you know what will be the you know input and output there that you can get it from this you know table it is summarized here as per this you have to do the you know summary for that after calculation for material balance and energy balance equation.

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Equipment wise Material Balance for Cumene Production from Benzene and Propylene

Equipment	Benzene column top		Benzene column bottom		Cumene distillation column top		Cumene column bottom		
	Distilled benzene		Feed to Cumene column		Cumene product		DIPB by-product		
	Mw	kmole	kg	kmole	kg	kmole	kg	kmole	kg
BENZENE	78	189.92	14813.84	0.00	0.00	0.00	0.00	0.00	0.00
PROPYLENE	42	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PROPANE	44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CUMENE	120	3.68	441.41	173.16	20779.60	173.16	20779.60	0.00	0.00
DIPB	162	0.00	0.00	5.59	904.92	0.00	0.00	5.59	904.92
TOTAL			15255.25		21684.52		20779.60		904.92

Now equipment wise material balance also for this you know benzene distillation column, even cumene distillation column, what will be the input and what will be the output, what is the top product, what is the bottom product it is given like this.

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Further reading.....

Text Books:

- R. M. Felder, Ronald W. Rousseau, Lisa G. Bullard, Elementary Principles of Chemical Processes, 4th Ed., John Wiley & Sons, Asia, 2017.
- D. M. Himmelblau, J. B. Riggs, Basic Principles and Calculations in Chemical Engineering, 7/8th Ed., Prentice Hall of India, 2012.

Reference Books:

- N. Chopey, Handbook of Chemical Engineering Calculations, 4th Ed., Mc-Graw Hill, 2012.
- Olaf, K.M. Watson and R. A. R. Hougen, Chemical Process Principles, Part 1: Material and Energy Balances, 2nd Ed., John Wiley & Sons, 2004.

So we have described here for this whole process of this you know cumene production with a target of 500 tons per day and for that, what will be the schematic you know process diagram, what are the different types of equipments are being used. And what will be the you know process variables for that, what are the you know process input, what will be the process output that has already been you know described here.

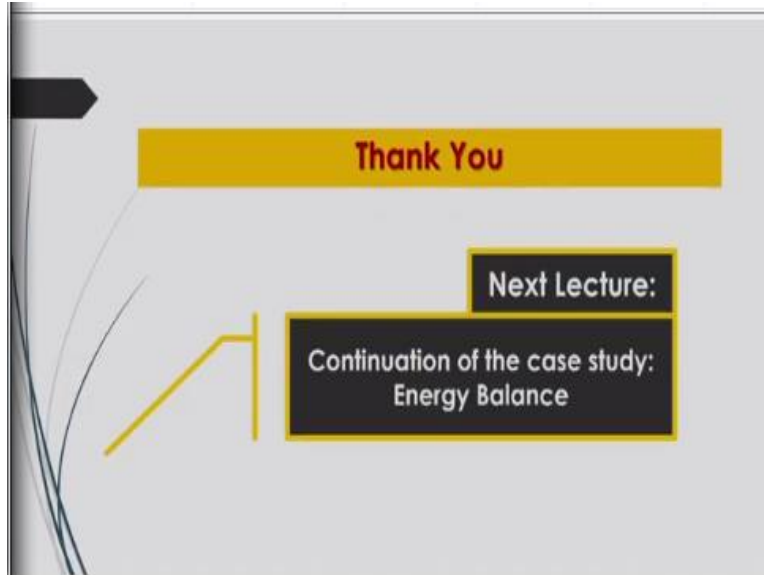
And what will be the amount of process input, what will be the amount of process output there. After each equipment you know what would be the output for that, what will be the temperature, what will be the pressure all these things here you know described. And accordingly we have you know done the material balance and then you can you know solve this material balance equation, and then get the you know input and output unknown variables there.

You can represent all those things in a you know that sequence of you know linear equation set for each equipment even you know combining all equations there and then solving, you can also be present in that way. So I think it will be helpful to you know calculate the you know input and output streams of that, you know industrial scale any process like this here, whatever described based on the material balance equation.

You can try yourself if suppose there is a target of you know 200 you know tons per day of cumene productions or 1000s ton per day cumene production remaining all other you know conditions are same there. Only thing is that your target will be changed then accordingly what will be the you know input and output for you know several equipments which are being used for this process that you have to calculate.

So I think you can you know practice it with a different you know target of that you know process output for the cumene production.

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So in the next lecture will try to you know discuss more about this process for energy balance . Here you will see that there are several units also are being used however you are changing the temperature of the processes streams with it is temperature. So accordingly how enthalpy would be changing for that inlet and outlet streams and based on that energy balance equation, you can calculate that in therapy for that inlet outlet streams for the several units there. So it will be discussed in the next lecture, so thank you for giving attention for this lecture.