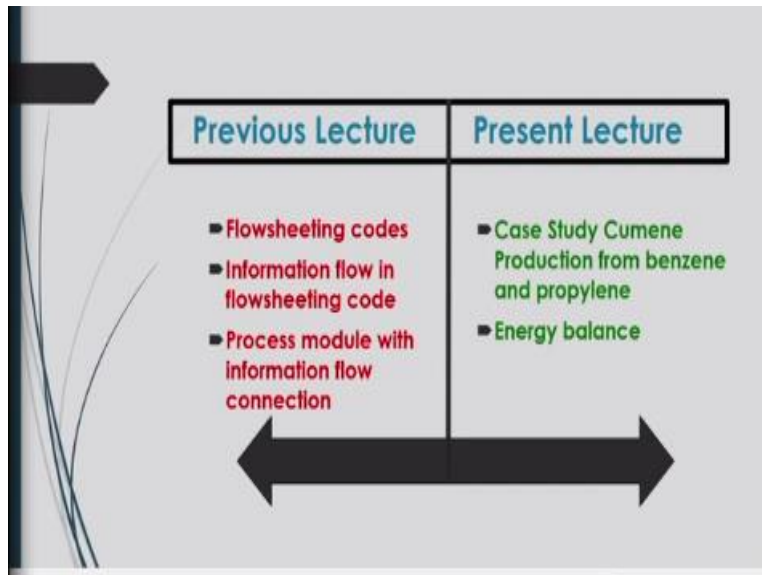


Basic Principles and Calculation in Chemical engineering
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Module-12
Lecture-35
Case study (continuation)

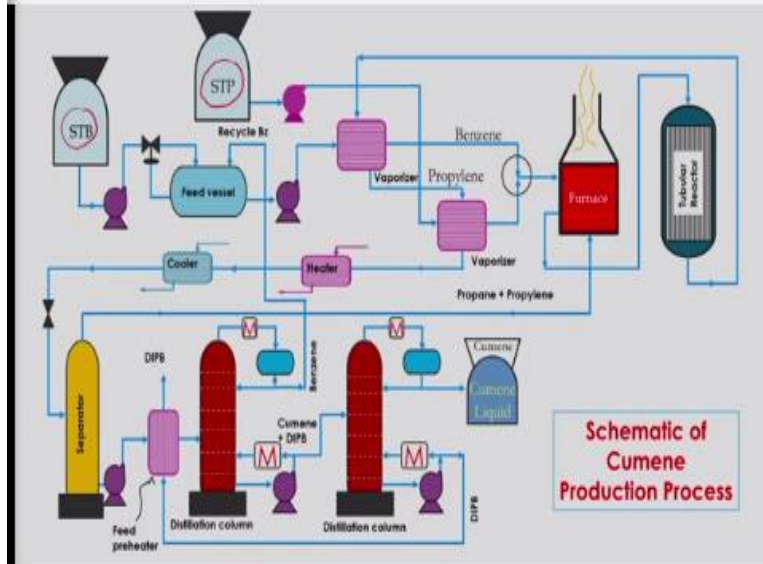
Welcome to massive open online course on basic principles and calculations in chemical engineering. Here we are actually discussing about case study for a process and in the previous lecture we have described the material balance of a chemical engineering process like Cumene production from benzene and propylene. And there we have described the material balance how.

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And what amount of different raw materials are required for individual equipments and for the whole process that we have described.

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Still you know go through again that process for you know describing the energy balance equation here in this lecture. So basically that Cumene is produced from the benzene and propylene at a certain you know temperature and pressure in a particular reactor. And then the product is being separated by you know different separator units like flash drum distillation column.

And before going to process those benzene and propylene for a reaction that benzene and propylene are heated up to a certain temperature of for its reaction. So here in this slides that description of the process with layout is you know shown when we have described it in previous lecture also. Now in this case basically these you know benzene and you know propylene those raw materials are coming from the storage tank.

And these you know benzene and propylene after heating up by vaporizer those are mixed and then it is again you know heat it up in a furnace to raise its temperature around 350 degree Celsius. For its reaction in the tubular reactor and in the tubular reactor generally the catalyst are being used as phosphoric acid that we have considered.

And then the output of that reactor is actually send to the separator through some vaporizer. However this outlet streams of reactor is utilize to heat up that you know benzene and propylene before entering to this reactor. And then outlet of those reactor and the fun is (()) (03:30) there.

So after that it will be send to separator so that in the separator the you know reactor products will be you know separated.

And that separation to be for just you know separating the unreacted you know materials that is taking parts in the reactions. Now unreacted you know materials are here propane and propylene also some amount of benzene will be there. So from the reactor these unreacted through propylene propane and you know benzenes along with that products like Cumene and the small amount of byproducts that is DIPV.

Those will be separated in a separator and there will not be only single separator because in a particular separator you cannot separate all the products at a time. So for that to separate the propane and propylene 1 you know flash drum is used as a separator where this propane and propylene will be you know separated and it will be you know utilized for heating purpose in the furnace.

And remaining that benzene DIPV and that is main Cumene will be reheated and then it will be send to one distillation column it is called benzene distillation column. However benzene streams would be you know separated from the mixture of that benzene, Cumene and I you know PV. And in this you know benzene distillation column from the distillate that you know benzene along with small amount of you know Cumene will be you know separated as a distillate product.

And those benzenes will be you know recycle to that feed basal of that you know fresh feed of benzene. And then it will be send to again to the reactor after vaporizing. Now from that benzene distillation column that Cumene and byproduct DIPV again it will be you know send to another distillation column which will be called as Cumene distillation column.

Now in that distillation column you will see that Cumene and DIPV will be separated from it is distillate and bottom parts. So, as a distillate to that Cumene has a liquid it will be coming after you know condensing and it will be around you know 99.9% as per that requirement of

production of this purity of this Cumene. And from the bottom part of this Cumene distillation column that 100% of DIPV will be you know taken out.

And it will be you know used for preheating or that you know mixer benzene DIPV and Cumene which is coming out from the separator of flash drum. And then DIPV you know used for other purposes. So, in this your whole process is actually going on for the production of 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.

Now, in the previous lecture we have described that you know what is the background of that reaction main reaction is basically propylene, benzene. And which will give you Cumene and byproduct with that propylene and Cumene will give you that di-isopropyl benzene.

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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

And different sections are here storage section, preheating section, vaporization section, pumping section and also reactor section there. And in the reactor section, the pressure up to 25 atmospheric pressure will be considered and the reaction will be done at 350 degree Celsius.

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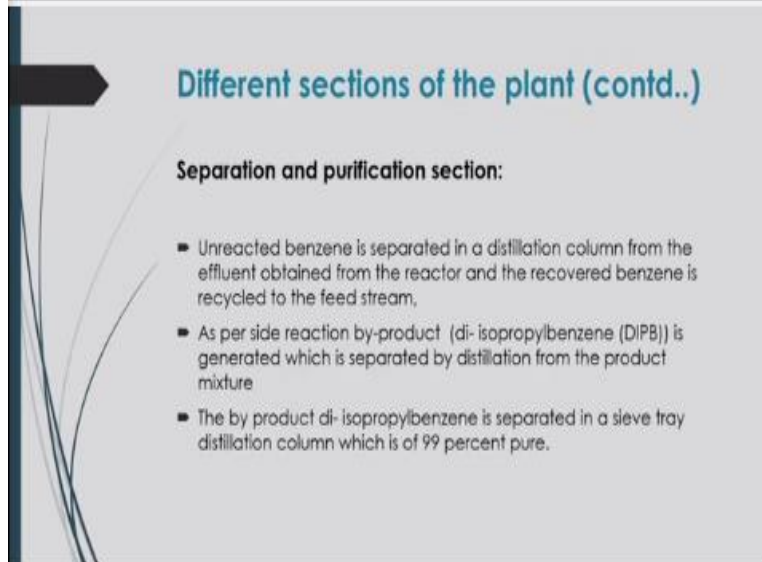
Different sections of the plant (contd..)

Reactor section:

- A tubular reactor is used to withstand the pressure up to 25 atm and 350 degrees centigrade.
- 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.

And from that after purification, we are getting that 99.9% of Cumene.

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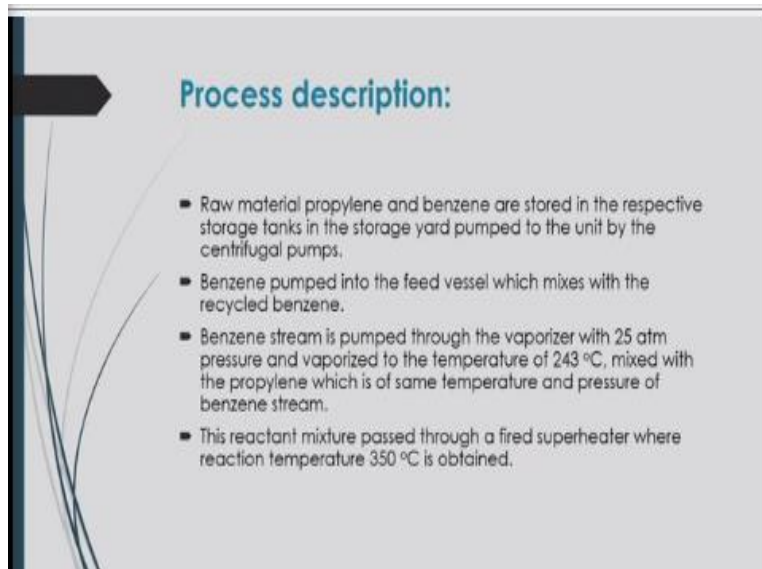
Different sections of the plant (contd.)

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, separation and purification section that involves that you know flash drum benzene distillation column and Cumene distillation column.

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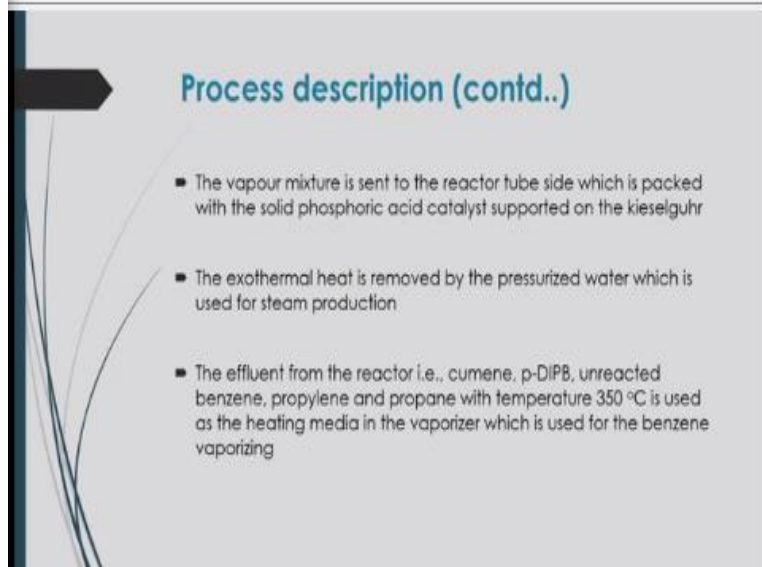


Process description:

- 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.

And we have described that process here.

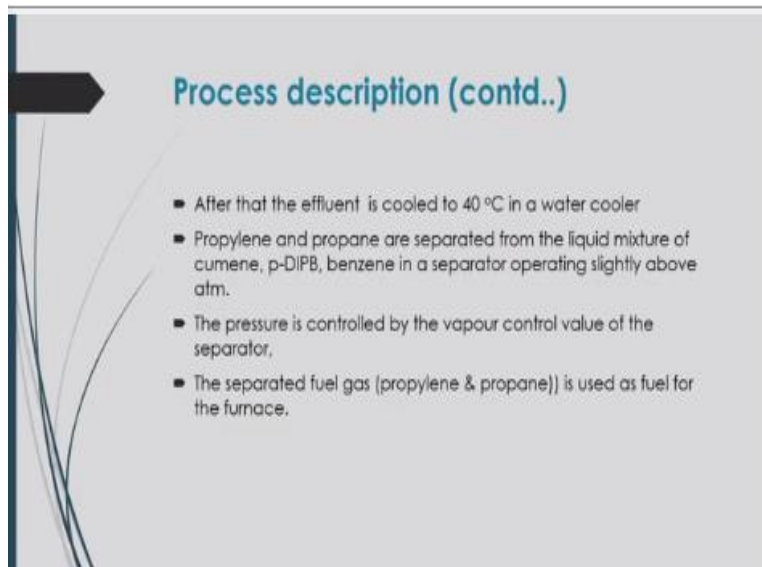
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Process description (contd..)

- 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

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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.

And then the details of that process description we have given in the previous lecture even also here, we have mentioned in the slides there.

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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

And in this case, you will see that.

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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

The overall material balance whatever we have done based on that you know mass conservation equation, that is described in our earlier lecture, what is the principles of material balance. And what is the governing you know material balance equations that we have described to us for those principles of that material balance we have done overall material balance.

And these overall material balance can be done for whole processes, if you are considering one single unit and what is that other unit separately there. So, for those cases you have to you know do the material balance, you can do overall material balance and also you can do the material

available balance for single unit or individual unit is separately. Now, in this case data assumptions are given.

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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.	

Here target is 500 tons per day of Cumene production, their conversion of propylene is 99%, product molar selectivity is 31 : 1. And propylene whatever it is being used that is 95% of purity remaining is along with that propylene is propane. And molar feed ratio of benzene to propylene to be maintained at 2 : 1. And top product of Cumene separation will be 99.9 mole percent Cumene and remaining 0.1% will be byproduct.

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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) + $\text{C}_2\text{H}_2\text{-C}_2\text{H}_2\text{-C}_2\text{H}_2$ (benzene) \rightarrow $\text{C}_6\text{H}_5\text{-C}_3\text{H}_7$ (cumene)
- Side reaction:**
 $\text{CH}_2\text{-CH}_2\text{-CH}_2$ (propylene) + C_6H_{12} (cumene) \rightarrow $\text{C}_3\text{H}_7\text{-C}_6\text{H}_4\text{-C}_3\text{H}_7$ (DIPB)

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

So, in this case based on this data assumptions we have done, that material balance by considering that reaction stoichiometry.

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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 ✓

And also the selectivity of that reactions are based on which we have calculated the you know what will be the amount of byproduct will be produced that is given here. It is around 5.59 kilomole per hour. As per you know assume data for production of Cumene.

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Inlet		Feed vessel	Outlet	
Fresh Benzene	178.75 ✓		Fresh Benzene	178.75
Recycle benzene	189.92 ✓	Recycle benzene	189.92	
Propylene	0 ✓	Propylene	0	
Propane	0	Propane	0 ✓	
Cumene	3.68	Cumene	3.68	
p-DIPB	0	p-DIPB	0.00	
Pressure	1	Pressure	1.00	
Temperature	40	Temperature	40.00	

Now if we consider that individual unit for this whole process is here and if we do the material balance we can get different you know composition of that inlet and outlet streams. Now if we consider that feed vessel or that benzene fresh benzene and you know, recycle benzene from the

benzene distillation column is mixed here. And then as a outlet it will be coming to the you know, that mixer where propylene will be mixed to this you know, mixture of these Benzene from these feed vessel.

So, according to that what are the different components first of all we have to know that they are we you know fresh benzene, recycle benzene you know that propylene, propane, Cumene you know para di isopropyl benzene. And what is the pressure and temperature. Now all those you know components to be considered for all the equipments individually.

So, in that case if we consider feed vessel what are the, you know fresh benzene is coming that is 178.75. whereas the recycle benzene that is coming from distillation column it is 189.92 as per you know balance equation. The details of that balance equation and the calculation is given in our previous lecture. So, we are not actually considering that details here again So, we are just summarizing for this here feed vessel you know inlet and outlet what will be the composition of different you know compounds there, so it is given.

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Inlet		Benzene vaporizer	Outlet	
Fresh Benzene	178.75		Fresh Benzene	178.75
Recycle benzene	189.92		Recycle benzene	189.92
Propylene	0		Propylene	0
Propane	0		Propane	0
Cumene	3.68		Cumene	3.68
p-DIPB	0.00		p-DIPB	0.00
Temperature	40.00		Temperature	243

Inlet		Propylene vaporizer	Outlet	
Fresh Benzene	0		Fresh Benzene	0
Recycle benzene	0		Recycle benzene	0
Propylene	186.20		Propylene	186.20
Propane	9.80		Propane	9.80
Cumene	0		Cumene	0
p-DIPB	0		p-DIPB	0
Temperature	25		Temperature	243

Similarly for benzene vaporizer propylene vaporizer, what are the different inlet and outlet compositions are given. So according to that calculation, you will see that at the same has already been discussed in details of that calculation given in the previous lecture. So, here just summarized that calculation, these are the things for mixer and furnace also it is given.

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Inlet			Outlet		
Fresh Benzene	178.75	✓	Fresh Benzene	0	✓
Recycle benzene	189.92	✓	Recycle benzene	189.92	✓
Propylene	186.20	✓	Propylene (unreacted)	1.86	✓
Propane	9.80	✓	Propane	9.80	✓
Cumene	3.68	✓	Cumene	180.52	✓
p-DIPB	0.00	✓	p-DIPB	5.59	✓
Pressure	25.00	✓	Pressure	25	✓
Temperature	350.00	✓	Temperature	350	✓

Similarly for reactor what are the you know fresh benzene is coming what would be the amount of recycle benzene is coming. And also you know profile in what would be the requirement for that propane along with that propylene what amount of that propane is coming. Cumene also a small amount it will come because the recycle benzene will contains that small amount of Cumene after separation in the benzene distillation column.

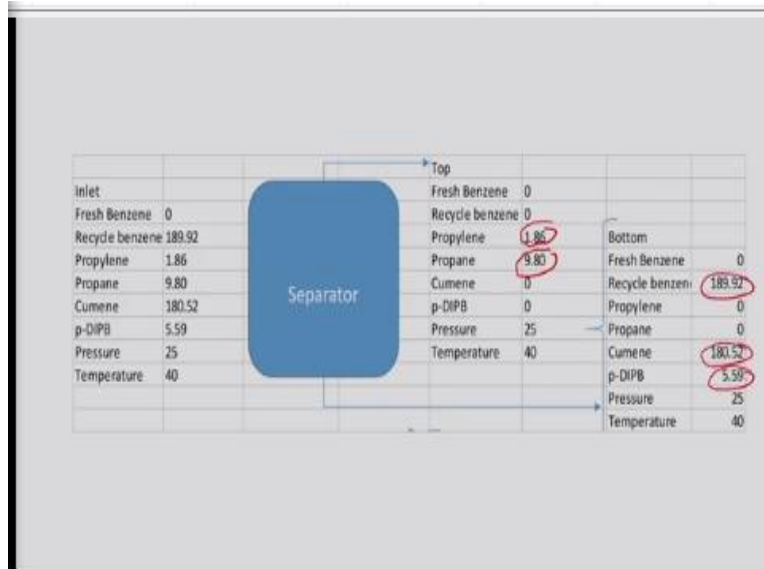
And then byproduct of course, will not be there in the you know reactor because 100% you know byproduct it would be you know separating out from the benzene distillation column and it is used for some other purposes. So, it is not being recycled there, and in the reactor the pressure will be you know 25 atmosphere and temperature will be 350 degrees Celsius.

Whereas from the outlet of this reactor the fresh benzene will not be there, because this benzene will be reacting and to be consumed. And you will see that as per that reaction stoichiometry and the conversion you can say that the unreacted benzene will be there that is will be coming out from the reactor, that will be 189.92 moles this is kilo moles.

And propylene also that will be unreacted that will be 1.86 and propane this is 9.80 which is coming along with that propylene. And Cumene after production this is the major amount here

this is 180.52 kilo mole. And a small amount of byproducts which will be coming out from the reactor and that pressure and temperature of 305 degree Celsius.

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And then it will be going to the separator from where you can say that top product of that you know separator will be coming. So you know that propylene and propane will be separated. Whereas in the bottom product that you know recycle benzene and Cumene and also you know byproducts will be coming out.

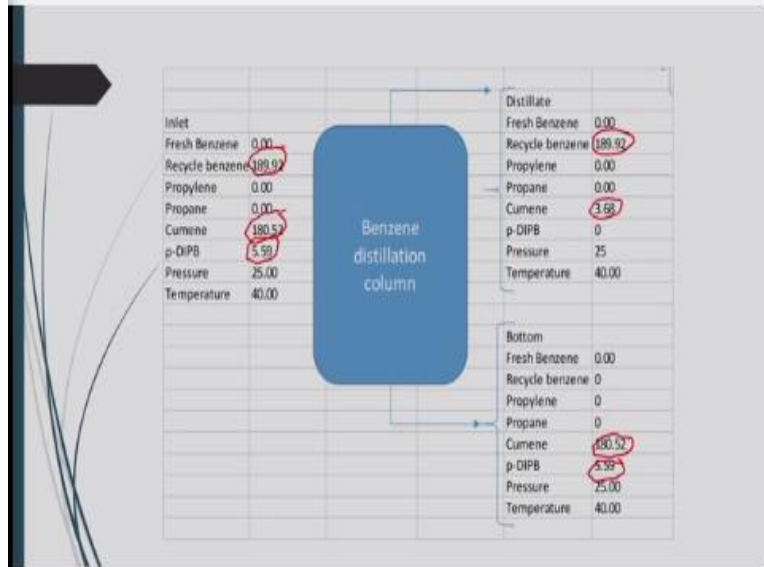
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And these are you know bottom product of the separator will go to the you know feed preheater the same amount and to be coming out also the same amount. But from the top you can say that

PIDP will be coming out because this PDIP will be used for you know heating purpose of this you know outlet of that you know separator. And then same amount of inlet of that feed preheater from the separated will be coming out from that feed preheater after preheating it.

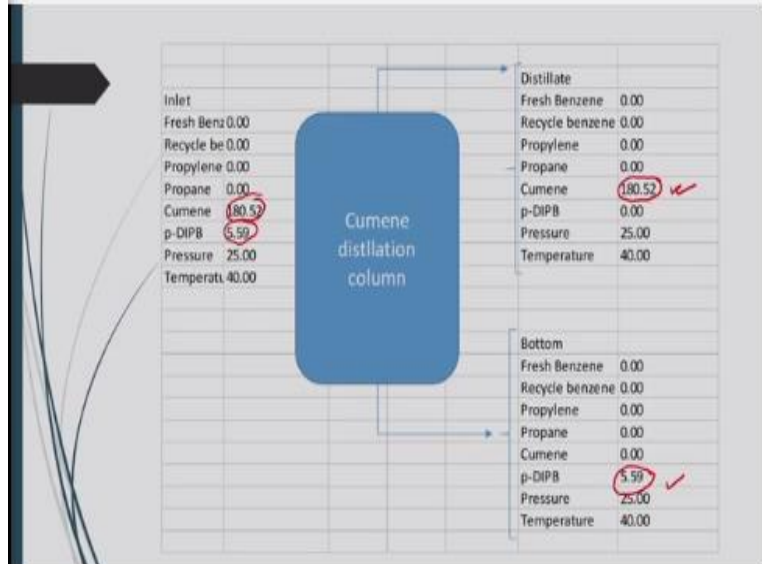
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And then it will be going to that benzene distillation column where you will see that only recycle benzene and Cumene and a small amount of p-DIPB will be separated. Whereas in the top product of this benzene and benzene distillation column it will be only recycle the benzene and small amount of Cumene. And the bottom product the main product that is Cumene will be coming out along with that you know byproduct there.

And then this bottom product of this benzene distillation column again to be separated in a Cumene distillation column.

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Where input of the Cumene distillation column will be the same that is Cumene and you know byproduct. And it is being separated and as a distillate on the you know that Cumene productive becoming. And at the bottom on that only you know p-DIPB will be coming. So, this final Cumene distillation column we are getting separation of this you know Cumene and byproduct.

So, we are getting here that you know desired you know purity of that Cumene and here that byproduct will be separated at a bottom product which will be used for preheating purpose. So, in this you have to tell procedure and the material balance and what will be the inlet and outlet proportions of that compositions are given here. Now, in this lecture main objective was to discuss that energy balance also.

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Equipment wise energy balance for 500 Ton/Day Cumene production pilot plant

- **For Benzene feed vaporizer:**
- The stream of mixed feed of benzene and cumene is feed to the vaporizer with 40 °C at 25 atm.

Component	Mol wt	kmole	Kg	mole fraction	mass fraction
BENZENE	78	368.67	28756.28	0.99	0.98
CUMENE	120	3.68	441.41	0.01	0.02
TOTAL		372.35	29197.69	1.00	1.00

In that case if we do the energy balance equipment wise for this process, we can say that for benzene feed vaporizer, if we consider first that because benzene will be send to the reactor after mixing with the you know propylene. And before that, those propylene and benzene will be you know vaporized to a certain temperature. Now these are to be vaporize to you know at 40 degrees Celsius.

Now the stream of mixed feed of benzene and Cumene is fed to the human vaporizer with a 40 degree Celsius at 25 atmospheric pressure. So there if we do the you know material balance there. We are having these benzene is 368.67 kilo mole, Cumene is 3.68 you know kilo mole, total this amount. Whereas more fraction of those components would be here 0.99, 0.01 and 1 as a total, and similarly for to the mass fractions.

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The bubble point and dew point of the mixture are found by using Antoine equation, the vapor pressure is calculated at various temperatures to find the saturated temperature

	p^v	x_i	$P = \sum p^v x_i$	$y_i = p^v x_i / P$	$y_i P$	$y_i P / p^v$
BENZENE	2587.64	0.990	2568.60	0.997	2562.07	0.990
CUMENE	660.50	0.010	2568.60	0.003	6.52	0.010
Σ		1.00		1.000		1.00

Where
 P = total pressure
 P^v = vapour pressure at 243 °C.

So, at 243 °C or 516 K the mixed feed will be vaporized.

Now, based on these you have to calculate in this you know vaporizer, what would be the vapor pressure of those you know components in this you know feed vessel of benzene. Now, the bubble point and the dew point of the mixer are found by using Antoine's equation. That means, how to you know get that you know bubble point from that Antoine's equation.

From those you have to first calculate to the you know that vapor pressure and from those vapor pressure what the respective temperature. That by that calculation you can easily get what should be the bubble point and dew point of that mixer by that Antoine equation. That Antoine's equation how to calculate already we have described in our earlier you know lecture. And then the vapor pressure is calculated at various temperatures to find the saturated temperature there.

And in that case the vapor pressure for the benzene for this more fractions it is coming 2587.64. And then Cumene is 660.50 as for data here, and then what will be the you know that partial pressure of that benzene here that can be calculated based on this air. And what will be the total pressure for that and what will be the more fraction of that, you know benzene accordingly **is** that can be calculated.

And partial pressure would be up for benzene is 2560.07 and partial pressure of Cumene will be 6.52. And here we can say that this p is basically a total pressure here this total pressure in this you know feed vessel. And p^v it is vapor pressure at 243 degrees Celsius. So, at 243 degrees

Celsius or 516 Kelvin the mixed feed will be vaporized there. So, it is called bubble point of this feed mixer.

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Heat required for vaporize	$C_p \Delta T$ + latent heat
Latent heat of benzene	23,773.63 kJ/kmole ✓
Latent heat of cumene	30919.2 kJ/kmole
Average heat capacity of benzene	161.46 kJ/kmole K ✓
Average heat capacity of cumene	246.92 kJ/kmole K

Enthalpy of benzene = $C_p \Delta T + \lambda = 161.46 \times ((243+273)-(40+273)) + 23,773.63 =$	56,550.01 kJ/kmole
Enthalpy of cumene = $246.92 \times ((243+273)-(40+273)) + 30919.2 =$	81043.96 kJ/kmole
Heat required for the mixed feed = $0.99 \times 56550.01 + 0.1 \times 81043.96 = 64088.89$ kJ/kmole = $64088.89 \times 372.35 =$	23863498.19 kJ

Now heat required for vaporized this basically one should be that due to the raise in temperature and also due to the feed change of that you know feed mixer. Now for that for feed change of course you have to consider that latent heat and for temperature difference that heat to be calculated based on that sensible heat like this is $C_p \Delta T$. So, heat required for the vaporize you know that it will be summation of that sensible heat and latent heat.

Latent heat of benzene here it is given that 23,773.60 kilo joule per kilo mole and latent heat of Cumene it is given here 30919.2 kilo joule by kilo mole. And average heat capacity of the benzene is given here 161.46 kilo joule per kilo mole k, k is the Kelvin here, it is here Kelvin. And average heat capacity of Cumene is given to 46.92 kilo joule per kilo mole k.

Now, what should be the then enthalpy that means heat required for the vaporization of the benzene, it will be simply sensible heat with you know latent heat that will be summation. So it will be coming as here sensible heat will be simply $C_p \Delta T$ is 161.46 it is given to you into no temperature difference is what is that earlier temperature is 40 degrees Celsius and bubble temperature is 40 to 43 degrees Celsius.

So, you have to subtract is this and before that you have to convert it to Kelvin, so it will be $243 + 273 - 40 + 273 +$ latent heat it is given here 23773.63 kilo joule per kilo mole. So finally the total amount is coming 56,550.01 you know kilo joule . Similarly enthalpy of cumene can be calculated based on that summation of sensible heat and latent heat as per this you know that sensible heat is like this and latent heat is this.

So, total amount of enthalpy for kilo mole of that Cumene is 81043.96 kilo joule per kilo mole. Now heat required for the mixed feed then it will be you know that what will be the fraction of those mixer of benzene and Cumene accordingly, that heat required for the mixed feed will be here, this is the percentage of that you know benzene into it is you know enthalpy of benzene it is given it is calculated as for this you know equation.

And also remaining is basically Cumene, so as per that we can get, you know that total amount of you know heat required for the mixed feed is like this 23863498.19 kilo joule.

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For Propylene feed vaporizer:

Propylene and propane fed from the tank	25 °C at 25 atm
The stream is vaporized and heat to the temperature and mixed with benzene feed.	243 °C
Bubbling point and dew point of the mixture is about	62.5 °C ✓
Latent heat of propylene	17229.4 kJ / h ✓
Latent heat of propane	17611.41 kJ / h ✓
The average heat capacity of liquid propylene	123.51 ✓
The average heat capacity of liquid propane	125.48 ✓
The average heat capacity of gaseous propylene	82.86 ✓
The average heat capacity of gaseous propane	97.48 ✓

For propylene feed vaporizer similarly you can calculate what should be the you know heat required for those. Now in this case propylene and you know propane fed from the tank is at 25 degrees Celsius at 25 you know atmospheric pressure. The stream is vaporized and heat to the temperature and mixed with benzene feed is at you know 243 degrees Celsius.

Now bubbling point and dew point of the mixer is about 62.5 degrees Celsius. Now latent heat of propylene is given here 17,229.4 kilo joule per hour. And latent heat of propane is given here 17,611.41 kilo joule per hour. And then average heat capacity of the liquid you know propylene is given is 123.51, average heat capacity of liquid propane is 125.48. The average capacity of gaseous propylene is 82.86, the average heat capacity of gaseous propane is 97.48.

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For liquid state		
	Propylene	Propane
C_p	123.51 ✓	125.48 ✓
ΔT (Bubble point-tank temp) (62.5-25)	37.5 ✓	37.5 ✓
Q (kJ/h) ✓	463.625	4705.5

For gaseous state		
	Propylene	Propane
C_p	82.86 ✓	97.483 ✓
ΔT (Final temp - bubble temp) (243 - 62.5)	180.5 ✓	180.5 ✓
Q (kJ/h)	14956.23	17595.681

And for liquid state, the C_p value for propylene is given 123.51 whereas it is for propane is 125.48. So, ΔT is basically that bubble point temperature and tank temperature of this propylene propane mixer and it is basically 62.5 – 25, then it is coming 37.5. And then what will be the heat required for that liquid state to raise this the temperature from 25 degrees Celsius to you know bubble point temperature of 62.5 degree Celsius.

So finally for propylene it is coming 463.625 kilo joule and you know that for propane it is coming 4,705.5 kilo joule. And for gaseous state for that you know propylene and propane you know after heating it you will see that it will be converting to you know gaseous state. Since it is mixed to that 243 degrees Celsius of course it is you know more than that bubble point temperature of that outlet stream of that benzene.

So there it is mixed of course immediately that propylene and propane will be converted into gaseous states. So, for that what would be heat they are to converting these you know liquid state

to gaseous state of that propylene and propane. So for that at that gaseous state that specific heat capacity of the propylene is 82.86 whereas it is for propane is 97.483.

And their temperature difference of course will be from that bubble point to that you know benzene feed temperature up to 243 degrees Celsius. Accordingly it will be coming as 180.5 degrees Celsius. So heat required for that it will be you know respectively for propylene and propane are 14956.23 and 17595.681 this is kilo joule per hour.

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Specific Heat required for component	Amount (kJ/kmol.h)
Heat required for propylene: (Liquid state heat + Latent heat + Gaseous state heat) = 17229.46 + 4631.625 + 14956.23	21861.08
Heat required for propane: Liquid state heat + Latent heat + Gaseous state heat = 4705.5 + 17611.39 + 17595.075	39912.5
Heat required for the feed: $196.00 \times (21861.08 \times 0.95 + 39912.57 \times 0.05)$	4461676.28

Now a specific heat required for component of you know that propylene, propane then we can say that heat required for the propylene how to calculate that total amount of heat. One is for you know when it will be you know temperature change from certain you know degree to certain degree Celsius at it is liquid state. And then converting that liquid state to the you know gaseous phase.

So their transition at that transition point of that you know liquid gas what will be the heat required that is latent heat. And again at that to gaseous state what will be the enthalpy change for that temperature change of the gaseous state. So, for that heat required for that propylene then finally we can say that after summing up all those whatever calculated here.

Based on which we can say that it will be total amount of you know 21861.08 kilo joule per kilo mole per hour. Similarly, heat required for propane similarly summation of that liquid state, sensible heat, latent heat and then gaseous state, sensible heat and summation of all those components that will be coming out as final amount as 39912.5 kilo joule per hour. And also heat required for the feed then accordingly what will be the total amount of moles for that propylene and propane.

Accordingly you can calculate here what will be the total amount of heat required for the feed, then it will be coming as like your 4461676.28 kilo joule. So, in this way we can calculate, you know that what should be the you know heat required for individual components for vaporizing it from a certain temperature to a certain temperature from liquid state to the gaseous state.

Similarly you have to do the energy balance for the fired heater also where these feed mixer of propylene and benzene to be heated up to a temperature of 350 degrees Celsius.

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For Fired Heater:
The heat required for raising the temperature reactant feed to 350 °C

Handwritten notes: $C_p = \int C_p dt$, 243 , 350 , 350 , 243 , 350 , 243 , 350

Compound	kmole/h	Heat capacity constants of gas mixture					Sp. Heat Enthalpy Cap.	
		A	B	C	D	E		
Propylene (C ₃ H ₆)	186.20	31.298	7.24E-02	1.95E-04	2.16E-07	6.30E-11	1.04E+06	1.93E+08
Propane (C ₃ H ₈)	9.80	28.277	1.16E-01	1.96E-04	-2.33E-07	6.87E-11	1.66E+06	1.63E+07
Benzene (C ₆ H ₆)	368.67	-31.368	4.75E-01	-3.11E-04	8.52E-08	-5.05E-12	6.77E+06	2.50E+09
Cumene (C ₉ H ₁₀)	3.68	10.149	5.11E-01	-1.77E-04	-2.26E-07	8.80E-11	7.29E+06	2.68E+07
Total								2.73E+09

Handwritten note: $Q_H = n C_p \Delta T$

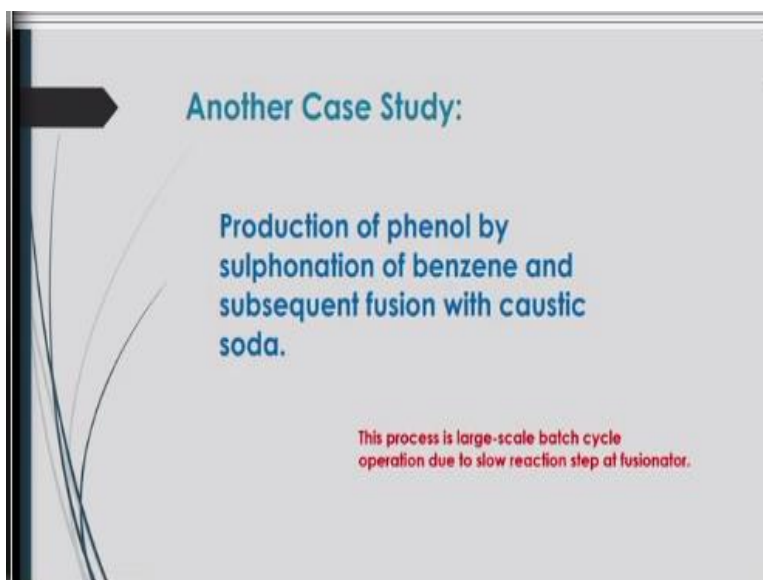
So, for that what would be the amount of heat required for raising this temperature of this reactant mixture of propylene and benzene to 350 degree Celsius. Now for that we have to calculate what from the enthalpy for that individual components of that mixture. So compound basically before going to that fire heater is you know that propylene, propane, benzene, Cumene all those things.

And they are respective flow rate that fire heater is already calculated based on that material balance. So, those amount are like this you know 186.20, 9.80, 368.67 and 3.68 respectively for you know propylene, propane, benzene and Cumene. And then you have to calculate what should be the specific heat capacity for individual you know components when that you know temperature will be changing from 243 degrees Celsius to 350 degrees Celsius.

Here, it is very interesting that this you know specific heat capacity will be a function of this temperature. Now how to be related this is basically related by this equation here given. That CP will be equal to $A + B t + C t^2 + D t^3 + e t^4$. So this is your you know specific heat capacity equation as a function of temperature. Now, based on these you know function you have to calculate what should be the specific heat capacity within a range of this temperature difference up to 243 to 350 degree Celsius.

Now, for that to what you have to do, you have to calculate in this way that a specific heat for this benzene it will be is equal to integration of this limit of this 243 to 350 degree Celsius of this you know for this here C p in D t. Now this will be coming as 243 to 350 C p here DT to be simply that C p is equal to a plus here BT plus you know C t square + D t cube + ET to the power 4 into D t.

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Another Case Study:

Production of phenol by sulphonation of benzene and subsequent fusion with caustic soda.

This process is large-scale batch cycle operation due to slow reaction step at fusionator.

And then you have to you know that integrate it within this you know limit of this integration and then you can get what will be the specific heat capacity. And for this A, B, C, D you know E all those are actually coefficients and these coefficients are you know varying according to the you know compound or nature of the compound. Now, for the propylene that coefficients are given here A, B, C, D, E respectively in this column here.

And similarly for propane these constants are given, for benzene also those constants are given, for Cumene also those constants are given. So, once you know these or substitute this you know this constants here in this integrant. And then do the integration you will see that after integration you will it will be coming as $80 + BT^2 + CT^3 + DT^4 + ET^5$.

And then you have to calculate the limit of this you know integrant to in this limit what will be the amount there. So, according to that for propylene it is the coming that here 1.04 into 10 to the power you know 6 this amount of specific heat capacity for propylene. Similarly for propane after integration it is coming 1.66 into 10 to the power 6 that means for propane.

Similarly for benzene it is coming 6.77 into 10 to the power 6, for Cumene it is come in you know 7.29 into 10 to the power 6. So, once you know this specific heat capacity within this range of temperature then based on this temperature difference of this 243 and 350 degree Celsius what should be the enthalpy. These enthalpy is basically, what is that for that gaseous mixer, so it is within that range of you know temperature change.

So, accordingly that enthalpy can be calculated simply what is that M that means here H will be or delta H to be calculated N into you know that C p here into delta t, so in this way you have to calculate. So accordingly this amount respectively for propylene, propane, benzene and Cumene can be obtained. And then total enthalpy after summation you can get it 2.73 into 10 to the power 9 ok.

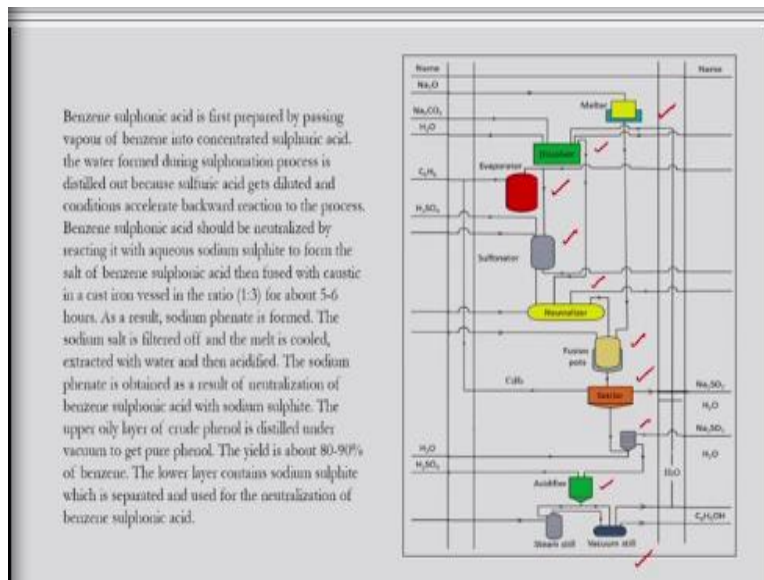
So, in this way you can calculate what should be the heat required for that particular you need to raise the feed mixer to it certain temperature for further processing. So we have described the

material balance and energy balance for the production of Cumene from the benzene and propylene based on their reactions. And also we have obtained that different you know, input and output streams compositions are based on that.

And also what should be the you know enthalpy change for that different components in the particular units that we can calculate and also we have given some you know calculations here. So, you can do the same way for other you know chemical processes for production of other you know compound there in a particular industrial scale operation. Let us do another case study here like production of phenol by sulphonation of benzene and subsequent fusion with caustic soda.

So, you can produce that phenol from the you know benzene by you know sulphonation process and also subsequent fusion with the caustic soda. This process is basically large scale base cycle operation due to slow reactions state for you know fascination of this you know benzene sulphonic acid with caustic soda.

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So, based on these principle we can you know have this you know process layout for this you know production of phenol. Now, let us discuss this process flow chart for this for this production of phenol from this. Like in this case you will see that benzene shulphonic acid is a first you know method to prepared by passing vapor of benzene into you know, concentrated sulfuric acid.

In that case the water formed during the self sulphonation process is actually distilled out because a sulphonic acid gets diluted and conditions accelerate you know backward reactions to the process. So mainly here benzene is reacting with the sulfuric acid and giving you you know benzene sulphonic acid and after that it will be you know neutralized and then you will see that it will be you know fused at you know a furnace with the you know that is caustic soda.

And after that you will see that some you know oily layer of crude phenol will be produced and then that oily you know crude phenol will be distilled under vacuum to get pure phenol and in this case the yield is about 80 to 90% of the benzene. So, what are the you know equipments are being used here for this process one is melter and one is dissolver and then evaporator, sulfonator, neutralizer, fusion parts or you can say that fusionator, settler.

And what is that you can say filter, acidifier and then you know that vacuum steel for distillation process. So in this case first of all you will see that some sodium oxide will be melted from it is solid to you know send to that fusion pots for the reaction with that you know benzene sulphonic acid. And before doing sending these you know sodium oxide there, sodium salt there what you have to do, you have to you know mixed with some sodium carbonate with water to make a solution.

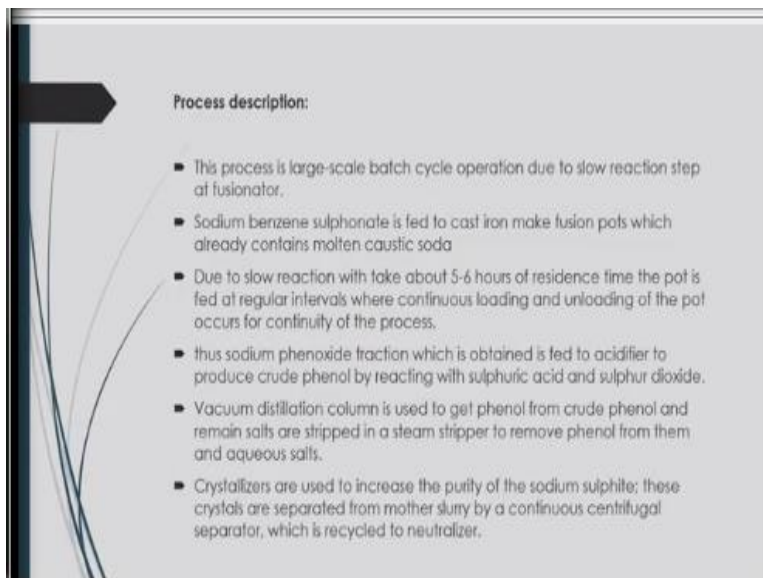
And that solution to be send to the neutralizer for it is neutralization, and in that neutralizer you have to send that you know sodium carbonate and sodium carbonate solution of you know along with that you know benzene. And you can say that you know that sulfuric acid there. And after neutralization you will see that those mixer will be sent to that fusion pots and however that sodium oxide will be reacted.

And then you will see that unreacted benzene and you know that sodium sulphate that will be formed during that fusion reaction. And also you will see that some you know water will be there extra water to be there. And to get that particular concentrated solution that water to be vaporized or distilled there. And also there is settler where that sodium salt will be you know that settle down and where the benzene will be you know, again recycled to it is fresh benzene feed.

And from that settler after getting that you know mixer of you know oily you know phenol, good phenol along with that sodium sulphate salt, it will be filtered out to separate that salt. And then remaining portion of crude phenol it will be send to you know vacuum distillation column. And they are it will be you know that distilled to get that you know some percentage of you know or purified you can say that phenol there.

So, this is the whole process here, so for this process also you have to do the material balance and also energy balance. And what should be the respective temperature of different units what will be different pressure at different units. And also what will be the inlet and outlet streams and what would be their composition and the amount that you have to find out by this material balance and energy balance equation.

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Process description:

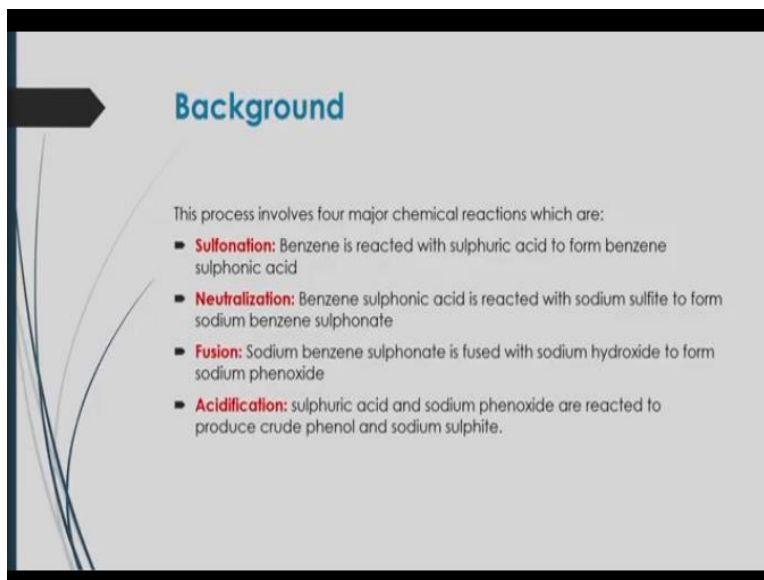
- This process is large-scale batch cycle operation due to slow reaction step at fusionator.
- Sodium benzene sulphonate is fed to cast iron make fusion pots which already contains molten caustic soda
- Due to slow reaction with take about 5-6 hours of residence time the pot is fed at regular intervals where continuous loading and unloading of the pot occurs for continuity of the process.
- thus sodium phenoxide fraction which is obtained is fed to acidifier to produce crude phenol by reacting with sulphuric acid and sulphur dioxide.
- Vacuum distillation column is used to get phenol from crude phenol and remain salts are stripped in a steam stripper to remove phenol from them and aqueous salts.
- Crystallizers are used to increase the purity of the sodium sulphite; these crystals are separated from mother slurry by a continuous centrifugal separator, which is recycled to neutralizer.

Now, process description that we have already described that this is the you know largest scale batch cycle operation due to slow reaction step at fusionator. Sodium Benzene sulphonate is fed to cast iron make fusion pots or who is already contains molten caustic soda there. Due to slow reaction with take about you know that 5 to 6 hours of residence time, the pot is fed at regular intervals where continuous loading and unloading of the pot occurs for continuation of the process.

The sodium phenoxide fraction which is obtained is fed to acidifier to you know produce crude phenol by reacting with sulfuric acid and sulfur dioxide there. Vacuum distillation column is used to get phenol from crude phenol and remain salts are strip in a you know stream stripper to remove himself from them and aqueous salts. Crystallizers are actually used to increase the purity of the sodium sulphite which is coming out from that you know (()) (41:46).

And these crystals are separated from mother slurry by a continuous centrifugal separator you can say which is recycled to you know neutralizer again. So, based on this process we are getting this phenol.

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Background

This process involves four major chemical reactions which are:

- **Sulfonation:** Benzene is reacted with sulphuric acid to form benzene sulphonic acid
- **Neutralization:** Benzene sulphonic acid is reacted with sodium sulfite to form sodium benzene sulphonate
- **Fusion:** Sodium benzene sulphonate is fused with sodium hydroxide to form sodium phenoxide
- **Acidification:** sulphuric acid and sodium phenoxide are reacted to produce crude phenol and sodium sulphite.

Now in this case the process involves 4 major chemical reactions, whose as sulphonation where benzene is reacted with sulfuric acid to form benzene sulphonic acid. Neutralization where benzene sulphonic acid is reacted to sodium sulfite to form sodium benzene sulphonate. And in the fusion reaction the sodium benzene sulphonate is fused with sodium hydroxide to form sodium phenoxide.

And in the acidification reaction sulfuric acid and sodium phenoxide are reacted to produce crude phenol and sodium sulphite and there it is you know separated.

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The reaction step explains the requirement of the unit operation equipment in the process as

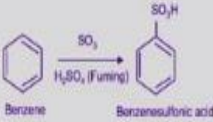
- **Filtration:** Pressure filter and centrifuge used in the separation of sodium sulphate and sodium sulphite
- **Distillation:** Separation of phenol from crude phenol
- **Crystallization:** Separation and recovery of sodium sulphite

That reaction step explains the requirement of the unit operation equipment in the process are here filtration and distillation and crystallization.

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Sulfonation of Benzene

- Sulfonation is a reversible reaction that produces benzenesulfonic acid by adding sulfur trioxide and fuming sulfuric acid. The reaction is reversed by adding hot aqueous acid to benzenesulfonic acid to produce benzene.



To produce benzenesulfonic acid from benzene, fuming sulfuric acid and sulfur trioxide are added. Fuming sulfuric acid, is a concentrated solution of dissolved sulfur trioxide in sulfuric acid. The sulfur in sulfur trioxide is electrophilic because the oxygens pull electrons away from it because oxygen is very electronegative. The benzene attacks the sulfur (and subsequent proton transfers occur) to produce benzenesulfonic acid.

And sulphonation of benzene basically is reacted based on this, this is reversible reaction. That produces benzene sulphonic acid by adding sulfur trioxide and fuming sulfuric acid. The reaction is reversed by adding hot aqueous acids to benzene sulphonic acid to produce benzene. Now to produce a benzene sulphonic acid from benzene fuming sulfuric acid and sulfur trioxide are added, fuming sulfuric acid is a concentrated solution of dissolved sulfur dioxide in sulfuric acid.

The sulfur in sulfur trioxide is electrophilic because the oxygen pull electrons away from it because oxygen is very electronegative. That is why it will be regarded as electrophilic reaction. And the benzene you know attacks the sulfur and subsequent proton transfers occur to produce that benzene sulfonic acid. So this is the mechanism how the reaction is taking place.

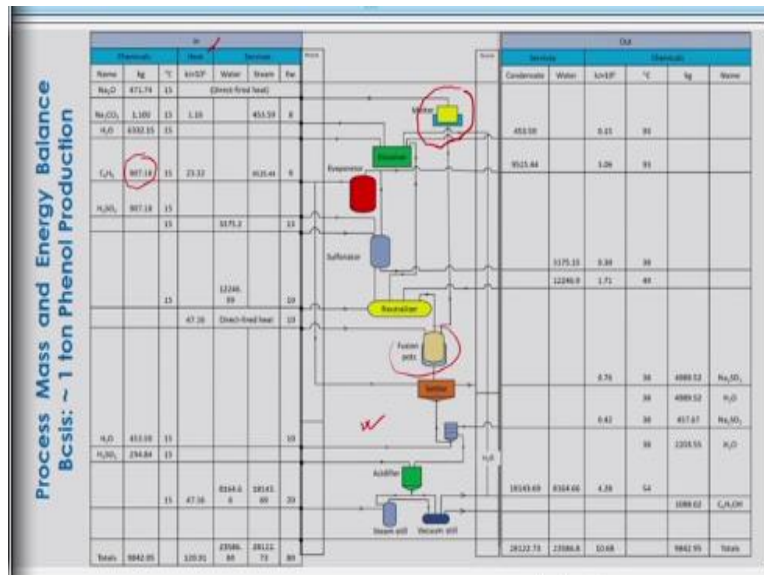
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■ Sulfonation of benzene is a reversible reaction.
 ■ Sulfur trioxide readily reacts with water to produce sulfuric acid and heat.
 ■ Therefore, by adding heat to benzenesulfonic acid in diluted aqueous sulfuric acid the reaction is reversed.

$$\text{C}_6\text{H}_5\text{SO}_3\text{H} \xrightarrow[\text{H}_2\text{SO}_4 (\text{Catalytic})]{\text{H}_2\text{O, Heat}} \text{C}_6\text{H}_6 + \text{HOSO}_3\text{H}$$

Now sulfonation of benzene is a reversible reaction that we know that sulfur trioxide readily reacts with water to produce sulfuric acid and heat. Therefore by adding heat to benzene sulphonic acid in diluted aqua sulfuric acid the reaction will be you know reversed, so this is your reverse reaction.

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Now here in this slides whole material balance and energy balance is shown here, see for equipment wise the material balance is being done. If we consider that melter here the what will be the you know chemicals are actually coming into this melter. It is basically sodium oxide and it is amount is 471.74. And as a outlet what would be the amount is coming into the fusion pots higher it is given the same amount it will be becoming after melting.

And then in this you know dissolver you see that sodium carbonate, the amount is given in kg here. And then here you know that water will be coming as you know there in the dissolver. And then you will see that after coming out from the dissolver you know that it will be going to that neutralizer there also what will be the amount of you know chemicals will be coming in basically this amount is coming here.

But before neutralizer there will be sulfonator there also you have to do the material balance here sulfuric acid coming this amount and benzene is coming here after evaporator. In this evaporator this amount of benzene is like this is kg. And then accordingly also other unit like what will be the inlet there and what will be the outlet there it is given there. So in the left side and the right side it is given inlet and outlet you know amount there.

So, we can say that at different you know unit we can do that material balance at accordingly what will be the inlet amount to be required for that you know particular you know basis of production of 1 ton of phenol there. So, here in this case you know fusion pots what will be the inlet what will be the outlet it is given, in the settler also what will be the inlet, what will be the outlet it is given.

Even in filter what will be the inlet and what will be the outlet is given there and acidifier also as per material balance what will be the sulfuric acid required also it is given. And what will be the outlet portion of that is given as per this from this acidifier. And also after that what will be the you know amount of inlet and outlet of this you know vacuum steel also it is given you know schematically.

And you will see that we have done also that you know that energy balance and accordingly what will be the heat required for that individual unit. It is given here as heat column you will see that different amount for different you know compound even different for unit. And also outlet also what will be the enthalpy that is at the outlet composition are also given.

And also inlet temperature of that is component what will be that and also outlet temperature what will be that it is given according to that calculation. And also what would be the outlet amount of individual compounds also given which is coming out from that individual unit all are calculated. And in this way also you can calculate for a specific chemical engineering process there and identifying that different units and reactions based on that reaction stoichiometry, what will be the input what will be the output.

And also you have to calculate that enthalpy based on that you know temperature change that is changeable heat and also latency if there any you know compound is changing from it is liquid state to the gaseous state. So please go through this you know slide here again for understanding that material balance and energy balance. And respective amount of you know heat and you know amount of stream at the inlet and outlet conditions and outlet streams there you can get it.

So, I think it will be very helpful for your further understanding of material balance for the particular process in industry.

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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. Chohey, 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, I suggest you to read further that this text book for your you know better understanding of different you know chemical engineering processes. And also their respective you know calculation based on material and energy balance.

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**Thank You
For choosing the course**

Wish you healthy and prosperous
life ahead.
.....All the best.....

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I would thank you for choosing this course and also I wish you healthy and prosperous life ahead. And of course all the best if is there any query please contact in this address email is given to this slides also website you can follow there accordingly you can mail me for further you know queries and also understanding. So I want to you know stop the lecture here, I welcome you to you know learn this course and also wish you healthy and prosperous life ahead and all the best, thank you.