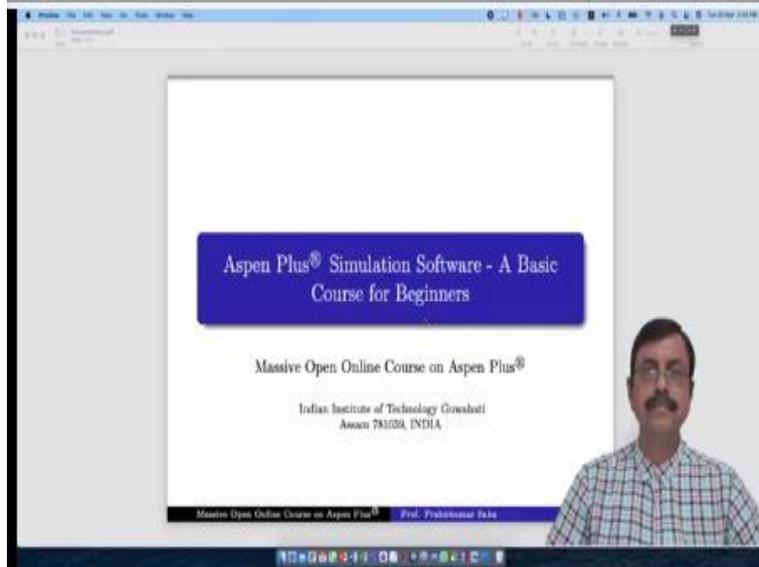


**Aspen Plus Simulation Software – A Basic Course For Beginners**  
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**Lecture-21**  
**Separation of Hydrocarbon Mixture**

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**Case Study – Separation of hydrocarbon mixture**

A hydrocarbon mixture of following composition

Component	Value
Hydrogen	31%
Methane	29%
Ethane	11%
Propane	11%
Hexane	13%
Heptane	8%
Octane	7%

is flowing at 120 kmol/h and at 30°C and 3 bar. The following tasks are to be performed.

- The mixture is to be flashed adiabatically with no pressure drop.
- The liquid line is the main product. First it has to be cooled down to 12°C with no pressure drop, and then it needs to be passed through a valve to decrease the pressure to 1 atm. The stream needs to be divided into two parts and sent to two plants in 80:20 ratio.
- The output of vapour line should be passed through membrane to separate into three streams, viz. hydrogen, methane (97% recovery) and all other hydrocarbons (mainly ethane-propane mixture).
- The ethane-propane mixture would be further passed through a separation column to separate ethane and propane.

*Handwritten notes: 'liq' and 'gas' with arrows pointing to the liquid and vapor lines of the flash process diagram.*

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In today's lecture, we will perform a case study on the separation of the hydrocarbon mixture. Now the hydrocarbon mixture separation is a prevalent instance in chemical and petrochemical plants. The hydrocarbon mixture that we have with us has the following components hydrogen 31%, methane 19%, ethane 11%, propane 11%, hexane 13%, heptane and octane they are 8 and 7%, respectively. Now all of them are in mole percent.

Now hydrogen and methane are light gases, and they always remain in the gas phase. Ethane and propane are medium range gas and can be liquefied, but the heavier components like hexane, heptanes, octane are always in liquid form at standard temperature and pressure.

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**Case Study - Separation of hydrocarbon mixture**

A hydrocarbon mixture of following composition:

Component	Value
Hydrogen	31%
Methane	19%
Ethane	11%
Propane	11%
Hexane	13%
Heptane	8%
Octane	7%

is flowing at 120 kmol/h and at 30°C and 3 bar. The following tasks are to be performed.

- The mixture is to be flashed adiabatically with no pressure drop.
- The liquid line is the main product. First it has to be cooled down to 12°C with no pressure drop, and then it needs to be passed through a valve to decrease the pressure to 1 atm. The stream needs to be divided into two parts and sent to two plants in 80:20 ratio.
- The output of vapor line should be passed through methylene to separate into three streams, viz. hydrogen, methane (97% recovery) and all other hydrocarbons (mainly ethane-propane mixture)
- The ethane-propane mixture would be further passed through a separation column to separate ethane and propane.

*Handwritten annotations:*  
 - P1, P2 (circled)  
 - light gas (pointing to H2 and CH4)  
 - fuel (pointing to C2H6 and C3H8)  
 - Ethylene (pointing to C2H4)  
 - isomers (pointing to C6H14 and C8H18)

After the separation, the hydrogen is expected to be purified to be used in the Syngas manufacturing plant. Methane is expected to be used as a fuel as in the natural gas, the ethane and propane can be sent for ethane, propane separator while ethane can be used for ethylene production and propane can be used to produce some isomers; there are plenty of applications possible I am giving just 1 or 2 examples. And finally, the hexane, heptane and octane they are the main products that we have and they need to be divided into 2 parts and sent to plant 1 and plant 2, so that is our main target.

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**Case Study – Separation of hydrocarbon mixture**

A hydrocarbon mixture of following composition:

Components	Value
Hydrogen	31%
Methane	19%
Ethane	11%
Propane	11%
Hexane	13%
Heptane	8%
Octane	7%

is flowing at 120 kmol/h and at 30°C and 3 bar. The following tasks are to be performed.

- The mixture is to be flashed adiabatically with no pressure drop.
- The liquid line is the main product. First it has to be cooled down to 12°C with no pressure drop, and then it needs to be passed through a valve to decrease the pressure to 1 atm. The stream needs to be divided into two parts and sent to two plants in 80:20 ratio.
- The output of vapour line should be passed through membrane to separate into three streams, viz. hydrogen, methane (97% recovery) and all other hydrocarbons (mainly ethane-propane mixture)
- The ethane-propane mixture would be further passed through a separation column to separate ethane and propane.

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Now the hydrocarbon mixture is flowing at 120 kmol/hr flow rate. Its temperature and pressure are 30 °C and 3 bar respectively. The combination is first, it should be flashed adiabatically with no pressure drop. So, if we have a flash tank, the feed will be divided into 2 lines: vapour and liquid lines. The liquid line is the main product. First, it has to be cool down to 12 °C.

So, whatever may be the temperature, we need to employ a cooler in the liquid line and the temperature is expected to be at 12 °C over here. And then it needs to be passed through a valve to decrease the pressure, so there will be a valve over here. At this end as there is no pressure drop and here it is 3 bar pressure. So, it is expected to be 3 bar pressure over here and that needs to be depressurized to 1 atmosphere at this end.

And then this stream needs to be divided into 2 parts and sent to 2 plants, so at this point it needs to be divided into plant 1 and plant 2 feed. It is in 80-20 ratio, so it will get 80% of the feed and 20% of the flow of the liquid line, so this is about the liquid line.

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**Case Study - Separation of hydrocarbon mixture**

A hydrocarbon mixture of following composition:

Components	Value
Hydrogen	31%
Methane	19%
Ethane	11%
Propane	11%
Hexane	13%
Heptane	8%
Octane	7%

is flowing at 120 kmol/h and at 30°C and 3 bar. The following tasks are to be performed.

- The mixture is to be flashed adiabatically with no pressure drop.
- The liquid line is the main product. First it has to be cooled down to 12°C with no pressure drop, and then it needs to be passed through a valve to decrease the pressure to 1 atm. The stream needs to be divided into two parts and sent to two plants in 60:20 ratio.
- The output of vapour line should be passed through membrane to separate into three streams, viz. hydrogen, methane (97% recovery) and all other hydrocarbons (mainly ethane-propane mixture).
- The ethane-propane mixture would be further passed through a separation column to separate ethane and propane.

Handwritten annotations on the slide include a process flow diagram with boxes and arrows, and labels for H<sub>2</sub>, CH<sub>4</sub> (97%), and C<sub>2</sub>H<sub>6</sub>.

And the vapour line, we have the output of the vapour line should be passed through the membrane to separate into three streams. So, we will have a membrane separator over here which will separate the vapour into three parts. The first will be hydrogen, the second one will be methane which is of 97% recovery, and all other hydrocarbons will go through the third stream in which there will be mainly ethane and propane mixture, so it will be ethane, propane mixture at this end.

And this ethane propane mixture would be further pass through a separation column to separate this ethane and propane. So, we will have another separation column over here, for that let us go to the Aspen plus simulation window. **(Video Starts: 06:15)** So, first we have to add the components, so let us write hydrogen, methane, propane, hexane, heptane, and octane. So, we have missed methane over here, so we have to add ethane because we have missed it, so say insert row and here you write ethane, now we have all seven components.

Now press next, now in the method filter, here we have common but as it is hydrocarbon mixture we can safely go and say that we want to use petrochemical processes. The relevant base methods only appear over here. So, these are the relevant base methods used in petrochemical methods and we shall choose the Peng-Robinson equation of state over here. Then press next and we have to run the physical property method. Yes, say it is done.

Now we have to go to the simulation block, so first we have to employ a flash tank, so flash is over here in the separator, so we have a two outlet flash at this point keep it over here. So, we rename it as flash and then we connect the material streams. There will be a feed, there will be a vapour line and there will be a liquid line. So, rename them, it is feed, then it is liquid, and this one is vapour.

Now let us press next, so we have to give the information about feed, so we know the mixture is flowing at 120 kmol/hr and 30 °C temperature, 3 bar pressure. So, we have 30 °C, 3 bar pressure and 120 kmol/hr flow rate. The components are in mole fraction it is hydrogen 31, methane 19, ethane, propane 11, 11. So, it is 0.31, it is 0.19, this is 0.11, this is 0.11 again, hexane 13, heptane 8 and octane 7, so 0.13, 0.08 and 0.07, so that makes it 1, the total mole fraction.

Press next, the flash again it is said that it should be flashed adiabatically with no pressure drop. So, adiabatic means there should be no heat duty, so heat duty is 0, so press duty 0 and pressure drop is 0, 0 bar means it is not at 0 bar pressure, it is not in a vacuum. 0 bar pressure means you might remember already I have explained 0 bar in Aspen it means pressure drop = 0,  $\Delta p = 0$  not  $p = 0$ , 0 or any negative value in pressure it means pressure drop. Now the flash is ready to run, just run it, so we can see the results, so this is the result we have.

So, we have mole flow out of 120 kmol/hr, 31.4 kmol/hr of liquid flows through the liquid line, whereas 88.563 kmol/hr of flow goes through the vapour line. So, individually we have almost the entire hydrogen goes through the vapour line. Only a tiny fraction of hydrogen remains in the liquid line. The same thing applies to methane and ethane as well, to some extent, propane.

But hexane, heptane and octane as I have said that they are mainly liquid at this temperature and pressure, and all of them go at the bottom, in the liquid line. So, this is the mole fraction we have, temperature and pressure are also given. In all the lines we have the same temperature and pressure and it is obvious because we have operated the flash tank in adiabatic condition and also there has not been any pressure drop in the line.

So, we go back to flow sheet and here one more thing that we will do, we will add some information icon on the flow sheet. For instance, if we want to know what is the temperature in these lines, we do not have to again and again go to the stream result. We can pick this temperature over here; it will display the stream temperature of the flow sheet. So, if we tick it you can see the feed temperature in the line has been given.

And here you will find the legend, you can see the legend over here, the temperature is like this. Now, if you want to see the pressure as well, it will show with a different icon, so this is pressure 3 is in the hexagonal block and in the oval block we have the temperature information. Similarly if you want to know the molar flow rate, you can tick over here, you see vapour is 89 and liquid is 31, total it is 120 kmol/hr, so this is the vapour stream.

Now the liquid line is the main product first it has to be cool down to 12 °C again without any pressure drop. So, we have to add in a cooler, we know that we have this heater or cooler the same block, so we add in the material stream over here and connect this. So, what we can do? We can choose this one, go to reconnect stream with a destination at this point, so this stream is connected, bring it over here it will look better.

And we have to rename it say cool liquid. So, we have to reduce the temperature, name the block as cooler, keep it over here or keep it at the bottom, this is a cool liquid, press next. Here they have asked the temperature and pressure. The information we have has to be cool down to 12 °C with no pressure drops. So, the temperature has to be 12 °C and there is no pressure drop, so it is 0 bar and then ready to run.

So, we can run over here, so run is complete and we can see that temperature over here is 12 °C, pressure is 3 bar because there is no pressure drop. And the flow rate remains at 31 because there is no other stream going in or out. Now you can keep another icon, heat or work, so this heat or work you will find over here  $q = 7547$  and the unit is it is in calorie per second.

So, this calorie per second needs to be thrown out if we have to reduce the temperature from 30 °C to 12 °C. And then we have to reduce the pressure, so we have reduced the temperature, now

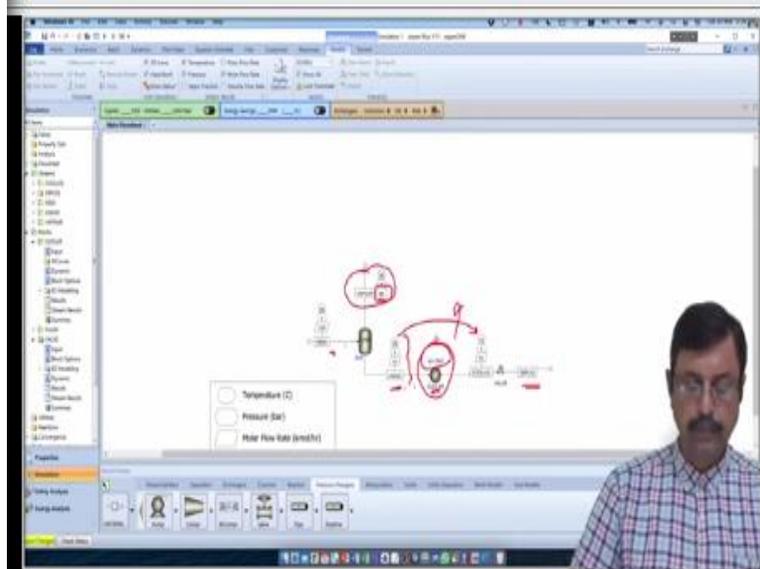
we have to reduce the pressure to 1 atmosphere by passing them through a valve. So, we have to bring in a valve over here, so pressure changer, keep a valve over here, choose this one, reconnect the stream to destination and material out, rename them.

So, write it as the valve, keep it over here, this is the one you can write it as liquid or depressurized liquid, DIPLIQ. And then press next, it will ask for the details of valve, so this is the valve input just keep it adiabatic flash or specified outlet pressure. So, outlet pressure we have to specify which is 1 atmosphere for our case. So, just keep it 1 atmosphere and you mind that we have valid phases vapour and liquid.

So, we have to keep valid phases vapour and liquid over here and in the cooler. In the cooler, if you see the input we have kept the valid phases to be vapour and liquid. Because unless we keep vapour and liquid both, if we keep only liquid then the system will give an error message in case it needs to be flashed. Obviously, it is in high pressure condition if you reduce the pressure from 3 bar to 1 atmosphere pressure.

In that case, definitely there will be a flash and some of the components will be vaporized and they will go at the top if you do not keep the option of both vapour and liquid as valid phases then the simulation will give an error message. So, you need to keep vapour and liquid phases both and as valid phases, so that is what is cooler. Now one more thing that you need to remember is that the cooler is needed at this point downstream.

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Because we need to cool down the liquid from 30 °C to 12 °C before we depressurized it because if we depressurize at this condition then a major amount of this liquid will be vaporized. Now you can ask the question why the cooler is given at the liquid phase? Why it is not given at the feed only? Because we do not want to unnecessarily cool 89 kmol/hr because cooler needs lot of energy reduction, so it needs power.

So, there is no need to cool down this 89 kmol/hr, so that is the reason we did not put the cooler over here. We have put the cooler just after liquid line, so that only that portion is cooled which is needed. Now this particular liquid needs to be splitted to 80, 20 ratio to be sent to 2 plants. For that we need a splitter, so we have this splitter, so just bring in the splitter over here but we do not like the icon.

So, we just change the icon, we do not like this icon either, no, we do not like it, this is not work, yeah. We like this icon very much, so this is a very good icon for splitter, so we connect this stream to the splitter. And then this is one line and this is the second line we have, we just bring it over here, so it looks somewhat better. Now here again we have to write splitter, so this is the block splitter.

And this is 2 plant 1 and this is 2 plant 2. Now again press next, so it is asking for the splitter input, so we know that we have to split in 80, 20 ratio. So, we just write that 80% will go to plant 1, so

we write 0.8 and do not have to give any information to P 2 because it has only 2 streams. So, if one stream is getting 80% of the flow then obviously the other line will get 20%, so you do not have to specify 20% again, it will take automatically.

Now the system is ready to run. So, run the system and your liquid line specification is complete. So, just go to the flow sheet, so this is the cool liquid, the heat duty in the valve is 0, so the depressurization happened from 3 bar to 1 bar and it is splitted between 2 lines TOP 1 and TOP 2. So, TOP 1 is getting 80% of the flow rate, so it is 25 out of 31 is going to the plant 1 and 6 kmol/hr out of 31 is going to the plant 2.

Temperature and pressure remains same that is 12 °C and 1 atmosphere pressure. So, this is about the liquid line. Now we have to work with the vapour line. So, about vapour line result, the output of vapour line should be passed through the membrane to separate into three streams: hydrogen, methane, which is about 97% recovery, and all other hydrocarbons, mainly ethane and propane mixture that will go into the third stream.

So, we have to use a separator, now membrane is undefined, we do not have anything called membrane separation in Aspen domain. So, if you are sure that you can write a code of your own that will define your membrane model, you can definitely choose the user model and bring it over here and connect your streams with this user model. Otherwise you can only take the separation, so it is component separator, it is of separates the component based on specified flows or split fraction.

In other words, you are not saying the underlying principle going on over there, whether it is a membrane or something else. You are saying that it is a common separator that is splitting as per your requirement. So, you know the final product, so in between some black box that is undefined but it is a separator, you know the final product. So, that is what it is. You just give it over here, connect this stream to this and here we have three streams, three-outlet streams.

So, this is the first outlet stream we have, this is the second outlet stream we have and we have a third outlet stream like this. So, just rename them, we write it as say membrane, so it is a membrane

separator for us. This one is hydrogen and this one is methane with 97% recovery and the last one is any other hydrocarbon but in principle they are ethane and propane. So, we can write as  $C_2$ ,  $C_3$ .

Other hydrocarbons are also there but mainly it is  $C_2$ ,  $C_3$  mixture which again we have to separate. Anyway, so our separator is defined, now we have to give the input of the separator, here we have very limited information. We know the membrane has to be separated into three streams, the first stream is hydrogen, so we can think of pure hydrogen. As if our membrane can separate one cut hydrogen which is pure 100% hydrogen.

The second cut will be methane which will have 97% recovery that means it will be pure methane but it will have 97% of the methane of the inlet stream that is coming to the separator. How is it done? What kind of membrane separation technique is used? Nothing is defined but you know the final product. So, this is methane, so first stream it is hydrogen, we say this is 100% hydrogen, the second stream we say it is 0.97 split fraction of 97% of recovery.

And the third one that is other hydrocarbons, we do not have to define because we already define 2 of them. The stream number 1 split fraction, stream number 2 split fraction we have defined. So, the third stream you do not have to define because it has defined by itself, out of 3 you have only 2 degrees of freedom. So, 2 degrees of freedom you have exhausted, the third one will be defined by the system itself, you do not have to define it anything.

So, if you want to define them forcefully, if you want to give some value to it say suppose if you go to this one and if you give a value. Then it will say consistency error in setting value that means you have defined hydrogen line and methane line, the other line you leave it to Aspen otherwise there will be consistency error. So, now the system is defined with the separator, just run and check.

So, you can see how things work, so out of 89, 37 kmol/hr, it is hydrogen, the entire hydrogen is going over there, then 22 out of the methane fraction is coming to  $CH_4$  line. So, if you want to check it once again, go to the stream result, here you will find the vapour line and the 3 streams that it has separated and you can see how much is the vapour. So, in the mole fraction or mole

flows you have 22.6835 methane in the vapour line, out of which 22.003 methane has come into the methane line.

Because you have taken 97% of the methane over there in the split fraction, the rest of it is going into C<sub>2</sub>, C<sub>3</sub>. So, here you do not have to fix anything, it has been already been fixed by itself. Now the last task remains for us the other hydrocarbons the C<sub>2</sub>, C<sub>3</sub> which is mainly ethane, propane mixture. It would further be passed through a separation column to separate ethane and propane.

Here again we have to use another separator, now again we can use this separator. But in this particular case we will use separator 2, where 2 outlet component separators separates components into two outlet stream based on flow and purities. Here in the separated column, if you see the input specification, you will find nothing other than split fraction and flow. But if you want to split it based on mole fraction and other things you have to use safe 2.

For that bring in safe 2 over here and then choose this one, reconnect with destination and then a material stream, this is one stream. So, choose this one to reconnect stream, source and then material stream bottom, this one. So, just take it and bring it down, so that we have some room for this one. So, we just rename it, we write it as say SEP unknown because we do not know what the technique behind this separator is? so separator unknown.

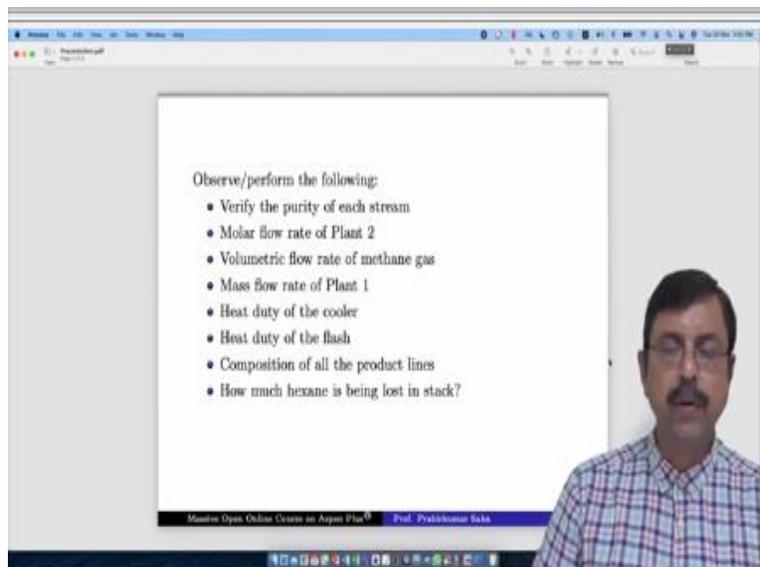
It may be a membrane, it may be something else but we know the end result. And this one we write C<sub>2</sub> and here we write C<sub>3</sub>. So, we know that C<sub>2</sub>, C<sub>3</sub> mixture will be separated into 2 streams. Now again press next, it will ask for the inputs for the safe 2 column, here you can find the outlet stream C 2, it is asking what the fraction of split fraction is? The first specification is bit the second specification is mole fraction or mass fraction.

So, here you can specify the stream with split fraction flow, so you do not have any first specification. Because you want the stream to go as per its own calculation, you want to tell the separator that this particular stream that is C<sub>2</sub> stream is at the top. So, it will have only the first four things if remains hydrogen, methane, ethane and propane hexane and heptane octane are not there because they are heavier products.

So, you write mole fraction 0, mole fraction 0 and mole fraction 0. So, this separator will not have any component of hexane, propane, octane. Similarly  $C_3$ , you will see that they are at the bottom, so it will not have any top component, so it will not have 0, 0, 0 and 0. So, run it, ok so it is run. Now here you can see the total is 29 out of which 25 has gone to the  $C_2$  column and it is  $C_3$  column, actually it is a misnomer.

Because we do not have  $C_3$  over here, all the  $C_3$  we have sent to this one, so we will write  $C_2$ ,  $C_3$  pure. And here we can write is a stack because this is the waste product that we are sending. So, so basically all the  $C_2$  and  $C_3$  ethane and propane we are sending it to  $C_2$ ,  $C_3$  pure and in the stack we are not placing any of them. So, only hexane, heptane or octane they are there in the stack. So, we have just changed the name accordingly, we write here  $C_2$ ,  $C_3$  pure and this is stack.

Now that completes the entire flow diagram and we have already run the system. We run once again because we have changed a few, now it is done. Now entirely you can check what is the pressure, temperature at each and every outlet? What are the flow rates at each and every outlet? And what are the heat duties in the respective unit operation? So, total, this separator, this separator, this cooler, and this flash, total the heat duty? You can find out. **(Video Ends: 43:24)**  
**(Refer Slide Time: 43:25)**



Observe/perform the following:

- Verify the purity of each stream
- Molar flow rate of Plant 2
- Volumetric flow rate of methane gas
- Mass flow rate of Plant 1
- Heat duty of the cooler
- Heat duty of the flash
- Composition of all the product lines
- How much hexane is being lost in stack?

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Now the next set of task is observe and perform the following. What do we have to observe or perform? First we have to verify the purity of each string. Now if somebody asks you what is the purity of each stream? Simply what you can do? **(Video Starts: 43:44)** You can go and check the results summary; there you will find streams and open all the streams. So, all the streams will be over here, so beginning from feed to vapour and liquid obviously they will not be of the order in which you want it but all the streams will be over here.

And this is very good because when you want to discuss it with your boss or with your team members, this kind of chart will be very helpful for you, you can explain it without just going here and there. If you want to know the pressure in some other unit, you just change it to say psi unit, so suppose if you want to converse with a person who is more comfortable in psi unit, we just convert it to psi and all the values in psi will be with you.

Or if somebody wants the heat duty or anything in watts and kilowatt in SI unit, you can write down kJ/kmol-K in entropy and so on. Now the first question is verify the purity of each string? So, for that purity means the mole fraction of the strings. So, this is the mole fraction, this entire unit is the mole fraction, this information. So, initially, we had mole fraction of hydrogen in the feed is 0.31, purity in hydrogen stream which is going through the membrane separator, it is 1.

Now there is no credit because we have given it that way, Aspen has just calculated. It has not done any calculation with membrane separator in mind but it has calculated as per the required information we have asked for. Now if somebody asks you what is the purity of say hexane in TOP 1? So, just go to result summary and choose the line TOP 1 and see the hexane, it is 0.398, so it is almost 40% of this stream will be hexane. Then molar flow rate of plant 2, so what is the molar flow rate of plant 2?

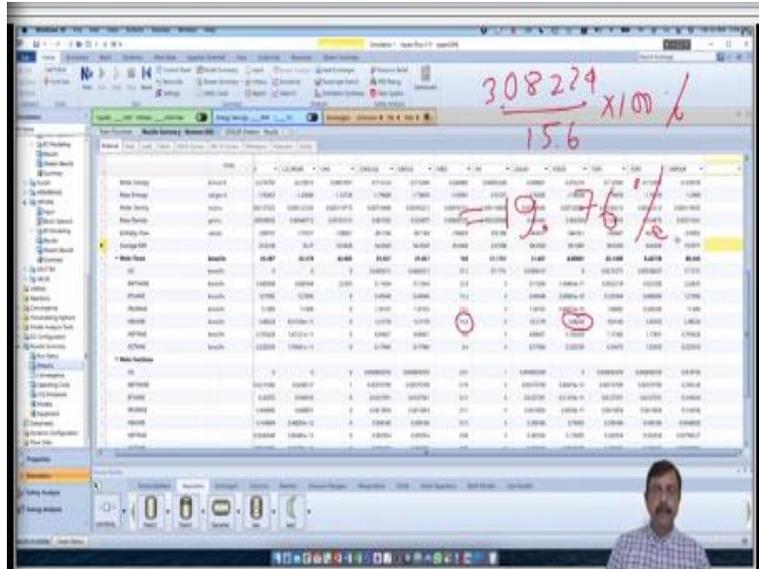
The same information you will get, plant 2 is here and the molar flow rate is 6.28739, this much of kilomole per hour is going to the plant 2, out of 120 kmol/hr feed then, the volumetric flow rate of methane gas. Now volumetric flow rate of methane gas you can see over here, volumetric flow of methane gas, methane is somewhere here it is in liters per minute, so 3061.7 liters per minute, you can convert it into say gallons per hour, it will be 48000 something.

Or if you want to use it as cubic feet or cubic meter per hour it will be 183. So, whatever unit you are comfortable with or your team members are comfortable with you can use them and you can show it better. Then the next one mass flow rate, mass flow rate of plant 1 feed actually it should be plant 1 feed, mass flow rate of feed to plant 1. So, this is TOP 1, this is the plant 1 and mass flow rate, so actually we are looking for mass flow rate.

So, it is 2380.58 kg/hr, so this is the mass flow rate to plant 1. Then heat duty of the cooler, again we do not have to go anywhere, we just see the flow sheet itself, the cooler heat duty is 7547. Now if you want to know the unit obviously if you have to go over there, unit is also written over here calorie per second. Now if you want to change it, you have to go to the, here in the results you can change it to kilowatt, it is 31.59 kilowatt, so that is the heat duty of the cooler.

The heat duty of flash it is 0 because we know it has been done adiabatically. And that can be corroborated with the information that we obtain. So, for that you do not have to go anywhere, just go to flow sheet and you will find the  $Q = 0$  over here in flash. Composition of all product lines, again this is the composition of all product lines over here and finally if somebody asks how much of hexane is being lost in the stack. So, that information is also over here, how much hexane is being lost in the stack? So, stack is over here and what is the hexane? Hexane is, so this much of hexane.

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So, it is 3.08224, this is so much of kilomole per hour of hexane is going through the stack. And what is the amount of hexane that was there in the feed? We had 15.6 that came to the feed line. So, how much is being lost? We have 3.08224 by 15.6 into 100, so much of percentage. So, if you calculate them, you will get it is around 19.76%, so this much of hexane is being lost in the stack.

Now it is up to the process engineer like you to decide whether this much loss of hexane is acceptable for this plant. In case you do not want to lose this much of hexane, you have to change the parameters that you are using in this plant, you have to change the pressure or temperature here and there; you have to change the heat duty. You have to do all sort of permutation combinations.

Obviously, it should be the educated way of doing it, not haphazardly or with any just wild guess. You have to do it with a certain plan and make it lower than 19.76 to the acceptable range, so that you can do without much problem. **(Video Ends: 53:28)**

So, we end our case study over here, thank you.