# Aspen Plus Simulation Software - A Basic Course for Beginners

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## Lecture - 09
## Example: Hydrocarbon Treatment- Part 1

Welcome to the massive open online course on Aspen plus. Today's lecture is a part of the lecture series to be taught in week 3.

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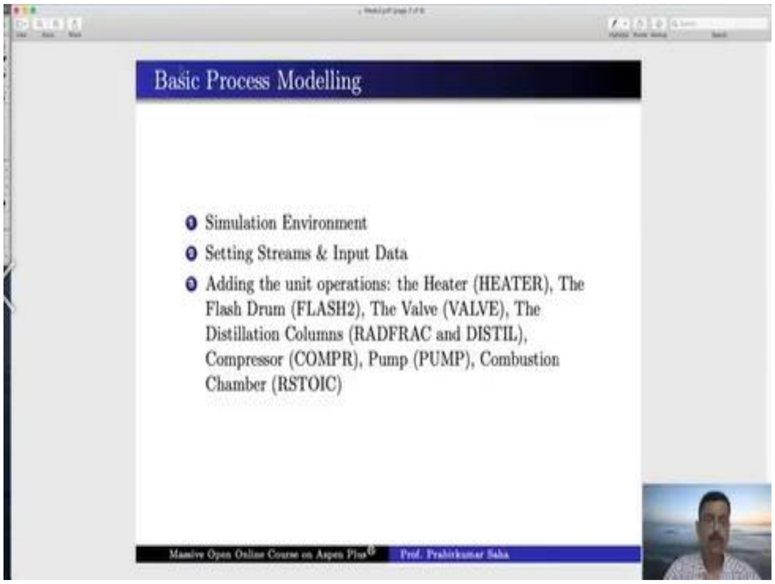

Basic Process Modelling

- Simulation Environment
- Setting Streams & Input Data
- Adding the unit operations: the Heater (HEATER), The Flash Drum (FLASH2), The Valve (VALVE), The Distillation Columns (RADFRAC and DISTIL), Compressor (COMPR), Pump (PUMP), Combustion Chamber (RSTOIC)

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We will learn the basic process modelling part which will contain the simulation environment setting streams and input data adding the input operations namely Heater, Flash Drum, Valve, Distillation columns to be very precise RADFRAC and DISTIL, Compressor, Pump and Combustion Chamber. The combustion chamber will be essentially a stoichiometric reactor. Now all of these unit operations, which I have mentioned right, are written over there on the slide.

They already have been discussed they have already been discussed in our previous few lectures. But today, we will learn them in detail. We will see how these unit operations can be set up in a plant-wide structure? How are they called from the menu? How are interconnected, and how the simulation is run on the entire plant-wide process? What would be the expected results whether it matches with the physical conditions? And then we shall analyse the result.

And at the end, we shall talk about some specific case studies that will necessarily be sensitivity analysis. And this sensitivity analysis will be based on the change in input variables to these processes, which we will discuss right now. First, we will talk about the problem statement. Now we will take the example of a hydrocarbon treatment process. Now, this hydrocarbon treatment process is a very common thing in petrol industries.

In hydrocarbon treatment, we treat hydrocarbon gas, which is essentially the mixture of various hydrocarbon gases, and then we separate them and get useful products out of it. The problem statement is something like this.

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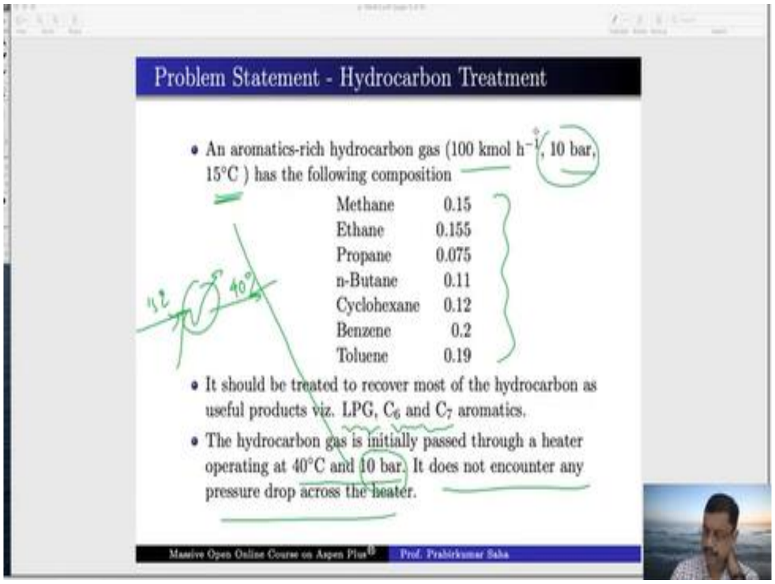

Problem Statement - Hydrocarbon Treatment

- An aromatics-rich hydrocarbon gas (100 kmol $h^{-1}$, 10 bar, 15°C ) has the following composition

| | |
|---|---|
| Methane | 0.15 |
| Ethane | 0.155 |
| Propane | 0.075 |
| n-Butane | 0.11 |
| Cyclohexane | 0.12 |
| Benzene | 0.2 |
| Toluene | 0.19 |

- It should be treated to recover most of the hydrocarbon as useful products viz. LPG, $C_6$ and $C_7$ aromatics.
- The hydrocarbon gas is initially passed through a heater operating at 40°C and 10 bar. It does not encounter any pressure drop across the heater.

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Aromatic, rich hydrocarbon gas whose flow rate is 100 kmol/hr and it is at 10 bar pressure and 15 °C temperature. They have the following composition. So, we have 15% Methane, 15.5% Ethane, 7.5% Propane, 11% n-Butane, 12% Cyclohexane, 20% Benzene and 19% Toluene. It should be treated to recover most of the hydrocarbon as useful products. What are the products?

LPG and Benzene and Toluene aromatics. So, these are the products that we are expecting out of the treatment. So, this hydrocarbon gas is initially passed through a heater operating at 40 °C and 10 bar. Now you see heater is needed to increase the temperature from 15 to 40 °C. So, if we have a heater, we will have the gas entering here at 15 °C, and it is expected to come out at 40 °C because the heater temperature is 40 °C.

And it does not encounter any pressure drop across the heater because it operates at 10 bar and the hydrocarbon gas is also at 10 bar. So, there is no pressure drop across it.

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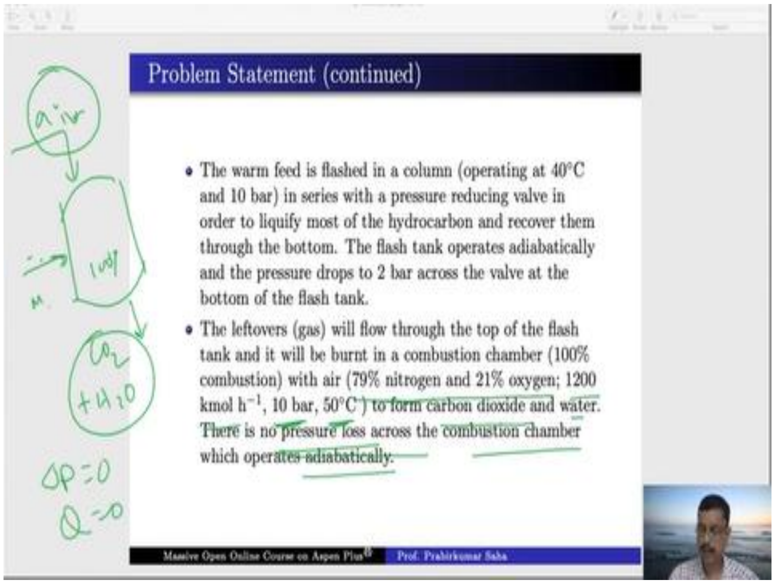

## Problem Statement (continued)

- The warm feed is flashed in a column (operating at 40°C and 10 bar) in series with a pressure reducing valve in order to liquify most of the hydrocarbon and recover them through the bottom. The flash tank operates adiabatically and the pressure drops to 2 bar across the valve at the bottom of the flash tank.
- The leftovers (gas) will flow through the top of the flash tank and it will be burnt in a combustion chamber (100% combustion) with air (79% nitrogen and 21% oxygen; 1200 kmol $h^{-1}$, 10 bar, 50°C ) to form carbon dioxide and water. There is no pressure loss across the combustion chamber which operates adiabatically.

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So, now this warm feed has already passed through the heater, so now it is warm. The warm feed is flashed in a column, so there will be a column somewhere after the heater. So, this is the heater output, so this will be flashed in this column operating at 40 °C and 10 bar, in series with a pressure reducing valve. So, if the temperature is constant then until and unless the pressure is released it will not liquefy.

There is no point in flashing them because flash means there will be a separation of vapour and liquid. For the liquefaction to happen, we have to reduce the valve and reduce the pressure through a valve. Now here it is 10 watt, pressure here it will be 2 bar because pressure drops to 2 bar across the valve. Now one more, information is there that the flash tank operates at operates adiabatically that means the heat loss or heat gain is equal to 0 across this column or flash tank.

Now the liquid has gone below, the vapour has gone above, so this vapour is called the leftover gas. So, the leftover gas will flow through the top of the flash tank, and it will be burnt in a combustion chamber. So, there will be a combustion chamber here. So, this is the combustion chamber, and to burn it to burn this leftover gas, we have to supply air because without air, the gas cannot be burned.

So, the combustion chamber is operated with 100% combustion. So, there will be no gas that is either methane or ethane or whatever there will be no trace of methane or ethane at the outlet. The outlet will be completely carbon dioxide and water. So, air will come with a composition 79% nitrogen and 21% oxygen, and it will have a flow rate of 1200 kmol/hr and here, it will have the pressure of 10 bar and 50 ℃.

So, this is the operating condition of the air. As I said already, it will form carbon dioxide and water, and there is no pressure loss across the combustion chamber that operates adiabatically. So, there are two pieces of information hidden here; no pressure loss and operates adiabatically.

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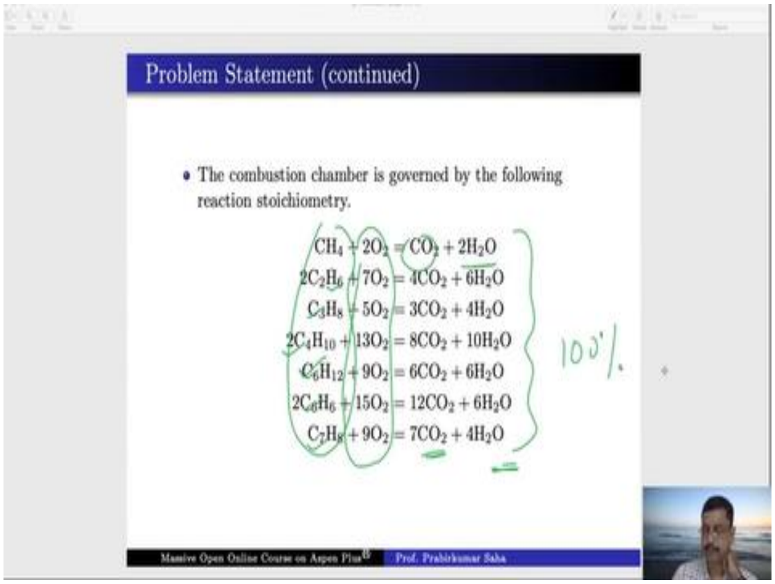

Problem Statement (continued)

- The combustion chamber is governed by the following reaction stoichiometry.

$$
\left.\begin{aligned}
CH_4 + 2O_2 &= CO_2 + 2H_2O \\
2C_2H_6 + 7O_2 &= 4CO_2 + 6H_2O \\
C_3H_8 + 5O_2 &= 3CO_2 + 4H_2O \\
2C_4H_{10} + 13O_2 &= 8CO_2 + 10H_2O \\
C_6H_{12} + 9O_2 &= 6CO_2 + 6H_2O \\
2C_6H_6 + 15O_2 &= 12CO_2 + 6H_2O \\
C_7H_8 + 9O_2 &= 7CO_2 + 4H_2O
\end{aligned}\right\} 100\%
$$

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Now here we find the combustion chamber. The combustion chamber is governed by the following reaction stoichiometry. So, these are the reaction stoichiometry. Methane is burnt with oxygen to form carbon dioxide and water. So are ethane, propane, butane, cyclohexane, benzene, and toluene. All of them are burned with oxygen to form carbon dioxide and water. They have their own stoichiometric proportions, but they all form carbon dioxide and water and mind that it is 100% combustion.

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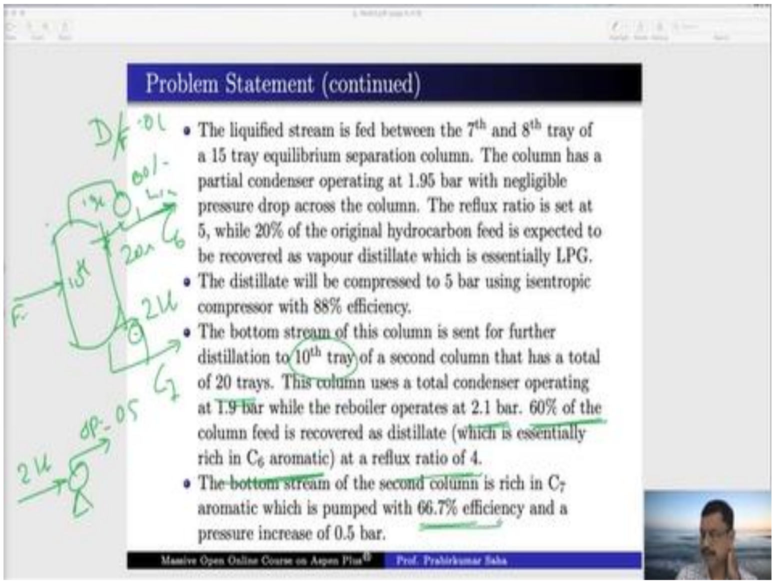

## Problem Statement (continued)

- The liquified stream is fed between the 7th and 8th tray of a 15 tray equilibrium separation column. The column has a partial condenser operating at 1.95 bar with negligible pressure drop across the column. The reflux ratio is set at 5, while 20% of the original hydrocarbon feed is expected to be recovered as vapour distillate which is essentially LPG.
- The distillate will be compressed to 5 bar using isentropic compressor with 88% efficiency.
- The bottom stream of this column is sent for further distillation to 10th tray of a second column that has a total of 20 trays. This column uses a total condenser operating at 1.9 bar while the reboiler operates at 2.1 bar. 60% of the column feed is recovered as distillate (which is essentially rich in $C_6$ aromatic) at a reflux ratio of 4.
- The bottom stream of the second column is rich in $C_7$ aromatic which is pumped with 66.7% efficiency and a pressure increase of 0.5 bar.

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Now we come to the bottom of the flash tank. So, top of the flash tank is leftover gas, we went to the combustion chamber—the bottom of the flash tank after it was passed through the valve where the pressure reduces and liquefied. Here, the liquefied stream is fed between the 7th and 8th tray of 15 tray equilibrium separation columns. So, there will be a distillation column where the stream is fed between the 7th and 8th tray of a total 15 tray column.

The column has a partial condenser at the top. A partial condenser means there will be vapour and liquid both in the condenser. And there will be a negligible pressure drop across the column, and the partial condenser operates at 1.95 bar. The reflux ratio is set at 5 which means if one mole of vapour is going out of the partial condenser, then 5 moles will come back to the column. So, the reflux ratio is set at 5.

While 20% of the original hydrocarbon feed is expected to be recovered as the vapour distillate, so, here it is 20% of the original vapour. So, what was original? The Original was 100 kmol/hr if you remember. If you remember, just a few slides back, it was 100 kmol/hr, 20% of that will be recovered as the vapour distillate, which is essentially LPG. Now this distillate will be compressed to 5 bar.

Here it was operating at 1.95 bar. So, it will be compressed to 5 bar using an isentropic compressor with 88% efficiency. So, this is the vapour distillate at 1.95 bar here it will be 5 bar LPG which will be recovered after the isentropic compressor. Now the bottom stream of this column is sent for further distillation. So, the bottom stream will essentially have $C_6$ and $C_7$, mostly benzene and toluene.

So, all the heavier keys will come at the bottom. So, this bottom stream will be sent for further distillation. So, this is the bottom stream and there will be a further distillation column here. The second column will have 20 trays, and the feed will be given at 10th tray. This column uses a total condenser. This is a total condenser which means there will be no vapour distillate, only liquid distillate. This condenser operates at 1.9 bar, and the reboiler at the bottom it operates at 2.1 bar.

60% of the column feed is recovered at distillate, so 60% of the feed means D to F ratio is 0.6. Now essentially, this is rich in $C_6$ aromatic so, this is $C_6$ aromatic. The reflux ratio is 4 that means if 1 mole of distillate is coming over here, 4 moles are sent back to the column. The bottom stream of the second column is rich in $C_7$ aromatic, which is pumped with 66.7% efficiency and a pressure increase of 0.5 bar.

So, there will be here there will be a pump. So, here it is 2.14, 2.1 bar and here it will be $\Delta p$ of 0.5 bar because of pumping and the pump operates at 66.7% efficiency.

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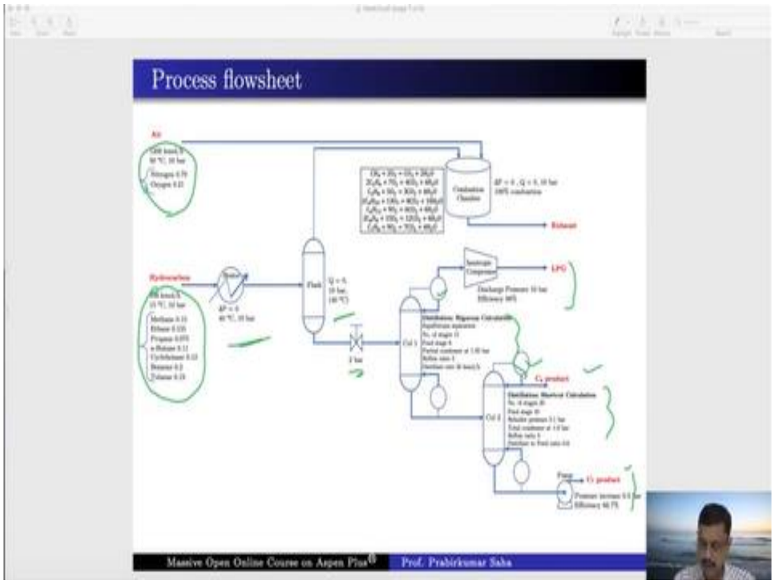

Process flowsheet

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Now here we have the complete process flow sheet in front of us. We can see all the unit operations discussed, namely the heater, flash tank, combustion chamber, column 1, column 2, isentropic compressor, and pump. The feed hydrocarbon is entering in the heater, whereas air is entering in the combustion chamber. So, the heated hydrocarbon is flashed where the major components are flashed and liquefied the leftover gas is being burnt in the combustion chamber. The first column it separates mainly the LPG and the $C_6$, $C_7$ components.

The LPG is being formed by passing the vapour distillate from column 1 through the isentropic compressor. While the bottom product of column 1 which are essentially $C_6$ and $C_7$ products, they are again passed through the column 2 and these are the condensers. These two are condensers. You can notice that this is the partial condenser. So, vapour distillate is coming over here, whereas it is a total condenser so, it is liquid distillate.

So, it is a liquid $C_6$ product, and here you find the $C_7$ product over here, which is coming out through the pump. Now here, all the specifications are written. So, while developing the Aspen plus model in the simulation environment or the property model, you have to define all these specifications you have to remember them, or you can take a printout of this flowsheet chart and then take the; you can form the model in the simulation environment.

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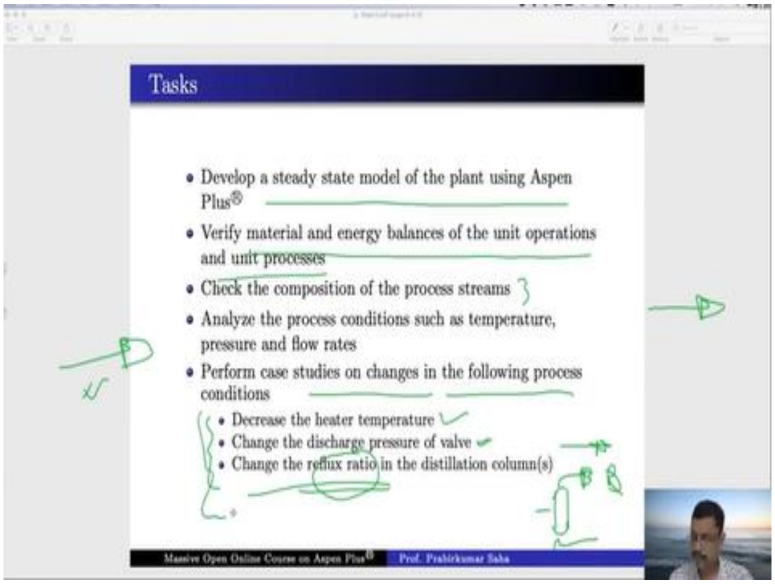

Tasks

- Develop a steady state model of the plant using Aspen Plus®
- Verify material and energy balances of the unit operations and unit processes
- Check the composition of the process streams
- Analyze the process conditions such as temperature, pressure and flow rates
- Perform case studies on changes in the following process conditions
  - Decrease the heater temperature
  - Change the discharge pressure of valve
  - Change the reflux ratio in the distillation column(s)

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Now what are the tasks that we have to do? First, obviously, we have to develop a steady-state model of the plant using Aspen plus. Then we have to verify the material and energy balances of the unit operations and unit processes. We have to check the composition of the process streams. The inlet composition definitely we have to set but the outlet composition which will be the result of the process analysis the process running of the process that we have to check.

Then analyse the process conditions such as temperature pressure and flow rates and perform a few case studies on the changes in the following process conditions. So, this we have identified for this case study. One is to decrease the heat heater temperature and see what happens, change the discharge pressure of the valve because the discharge pressure of the valve decides how much liquefaction will happen after the flash tank.

And finally, we will change the reflux ratio in the distillation column and see what would be the results of the change in reflux ratio. Basically, the distillate condition will depend upon the reflux ratio. That is the purity of the distillate. So, we will see all of them. Now let us go to the simulation environment now.

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So, the Aspen plus is opening. We have to give it some time. So, the Aspen plus has been opened. Now we have to develop we have to open a new flow sheet. So, it is a blank simulation and will run create. So, first we have to add in the components. What are the components do we have? Let us see, so we have these components methane, ethane, propane, n-butane, cyclohexane, benzene and toluene.

So, we have to add in these components one by one. Let us write methane. These are the conventional thing conventional chemicals. So, if you write methane, it will understand you are looking for $CH_4$. So, methane it will understand ethane, propane, and also will it will understand n-butane very common, but cyclohexane it may not because see it has a very limited only 7 letters are available for defining your component ID.

So, cyclohexane it may not understand what it is if you write if you write cyclohexane, it may not understand. So, it is writing conventional, but it does not identify anything like the ones we have already defined. So, what we can do is, we can say find so here we will write cyclohexane as full and we will say find now. So, it will search, yes. Now it has searched so many items which are similar to the term cyclohexane that we have written.

Now, this is the one which we are looking for $C_6H_{12}$. So, we will say add the selected compound. Once we do it, you can see it has added ‘cyclohex’, which could not find the component name it has added. The other two are very simple benzene and toluene so we write it in this fashion it will accept. Now we have to press next and we have to see what are the property methods that we can use.

Now we have a method assistant we can take the help of a method assistant. If you know what method, you should use you can directly look for it otherwise you can take the help of method assistant. So, this is the method assistant property method assist selection assistant you have to specify component type it is a hydrocarbon system. Does the mixture contain petroleum assay or pseudo component? Yes, it has. In the system is vacuum condition, no.

So, you can use these methods use Chao-Seader cedar or GRAYSON if the system contains hydrogen, but our system does not contain hydrogen. So, you can use Braun K-10 or an equation of state methods such as Soave-Redlich-Kwong and Peng-Robinson. Now let us choose the Peng-Robinson method. So, the base method is Peng-Robinson. Here, you can modify the equation of state method liquid molar enthalpy molar volume etcetera heat of mixing if you have.

So, you can modify your Peng-Robinson method based on some extra data that you may have. We do not have any such data so we can just go forward with next. Then it will quickly calculate the binary interaction temperature-dependent binary interaction methane with ethane methane with propane methane with n-butane ethane with propane ethane with n-butane propane with n-butane and so on.

So, all these temperature-dependent binary parameters will be calculated for you. Now these property methods are there, we have the property result. Now we have to go to the simulation environment. So, we press the simulation environment it comes here. Now the first simulation we have to add a heater. So, go to exchanger this heater thermal and face state changer model heaters coolers condenser etcetera.

So, let us use this heater. We have to give it a name so, let us name it heater, press it here and then it should have material input feed, and this is the product. Now here we have to rename it say hydrocarbon. We rename it, and then we press ‘Next’. So, these hydrocarbon inputs we have to give. So, what is the temperature and pressure? It is 15 °C and 10 bar. So, it is 15 °C and 10 bar pressure and flow rate 100 kmol/hr.

So, we write 100 kmol/hr. Now you have the option to give in other units but we have kilo mole per hour unit over here with a mole basis. So, we are using this directly. We can give it in mass base or volume base also. Now composition we can give individual mole flow but we have it in the mole fraction so, we have to write mole fraction. Then methane 15% ethane 15.5 so, we write 0.15, 0.155.

So, as you keep on increasing, if as you keep on typing the total mole is coming the total mole fraction is coming over here. Now it should reach 1. So, propane 0.075, n-butane 0.11, so it is 0.075, 0.11. cyclohexane 0.12, benzene and toluene 0.2 and 0.19. cyclohexane 0.12, 0.2 and 0.19. So, the total is 1. So, we are ready with the input go to next it opens the heater input block. So, here again heater there are three information available that is 40 °C, 10 bar pressure or pressure drop to be 0.

Now here temperature, we give 40 but pressure if you give 10 bar, the pressure will be taken.
If you give it 0 bar it does not mean the pressure is 0 or vacuum it means the pressure drop is 0. And if you give -1 that means the pressure drop is -1 any negative or 0 will be regarded as pressure, drop while any positive value will be regarded as the absolute pressure. So, the moment, I give 10 bar the specification is complete with a blue tick.

Now we write next, now all the required inputs are complete so we can run the simulation now. So, please run it will run the simulation and it will give you the sequence of messages processing input specifications. So, calculations begin heater simulation calculation completed with no warning no error. It is quite understandable because our flow sheet did not have any complication. We have a feed that is being heated within a heater.

Now here we can see the result, double click and you will find the material result. So, the outlet will have a temperature of 40 °C because heater is maintained at 40 °C. This is the pressure now as because pressure has been increased so there are certain vapour fraction and liquid fraction of the entire thing based on the particular pressure and temperature and that pressure and temperature some of the content will be in a liquid form. So, that is what it means.

Now we have to add a flashover here followed by a valve. So, flash we will use this so two outlet flash this is two outlet flash and this is three-outlet flash. So, we have two outlets so we will use this flash 2 followed by a valve. So, valve is there in the pressure changer so we will keep the valve over here and come back to the material choose this one this material reconnects the stream destination this one.

Then this stream will be connected to this this will come out here and this will come out like this. Now we have to specify already 2 is specified as it is the heater output but the flash and the valve, we have to rename first so this one is we write it as FLASH and we write it as VALVE. Now they are not defined because we have to give the operating conditions in the valve and the flash. So, press ‘Next’ here the flash input let us see there are three inputs available.

It is adiabatically there is no temperature loss heat duty is 0, pressure is 10 bar or 40 °C. Now we have to choose any two of them because it is asking any two between temperature due to vapour fraction and here between pressure due to vapour fraction. So, we shall choose these two that is Q is equal to 0 and 10 bar. So, we will choose heater duty which is 0 and pressure is 10 then it is blue ticked. Next it will ask for the valve condition.

The valve will be operated at 2 by the pressure released at 2 bar. So, we write as 2 bar outlet pressure 2 bar then it is ticked. Then again run the simulation we can run it again no error no error no error no error no warning and we can see the composition of the leftover gas. These are the composition of the leftover gas. So, we will see 30 moles, 30 moles have come out. Rest of the things will go down if you compare 4 with 5 you see 30.566 kmol/hr this is the leftover gas and this is 69.433 kmol/hr, total will be 100 kilo mole, is not it.

So, 4 and 5, there 4 this is 4 and this is 5 so, this is 30.5667 kmol/hr this is 69.4333 kmol/hr and this is 100 kmol/hr. So, this was it is, total is 100. Now this is going to the column 1, now here we will have a rigorous calculation of distillation. So, for rigorous calculation we will use a column with Radfrac it is for rigorous two or three phase fractionation in distillation column single column. So, we choose Radfrac and the top of the distillate will go to isentropic compressor.

So, we choose again go to the pressure changer, bring this compressor over here and connect with the material streams. So, reconnect destination here then here there are two outlets, this is for vapour distillate and this is for liquid distillate. Now we have vapour distillate over here because vapour will be compressed and to form LPG. So, we take vapour distillate connect to this and this will be our LPG and this will be the bottom product which will be essentially the mixture of $C_6$ and $C_7$ products aromatics.

So, to make the thing a bit better we can keep it here and bring it over here. It will look better it does not matter with the calculation but just for the ease of simulation we keep it over here.
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