Aspen Plus Simulation Software - a Basic Course for Beginners

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Lecture - 10
Example: Hydrocarbon Treatment- Part 2

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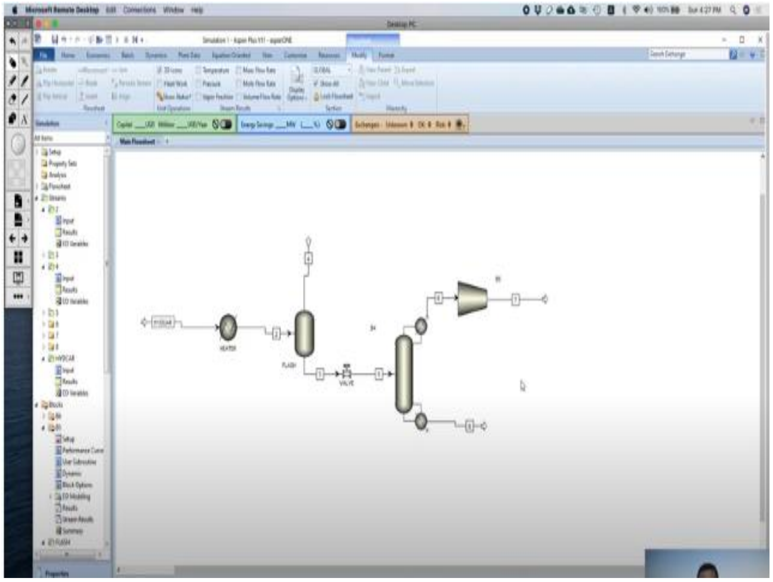

Now we must rename this compressor. Let us say we write it as a compressor. It does not take more than 8 letters. So, we must make do with compress. Now we must write the specification of the compressor here.

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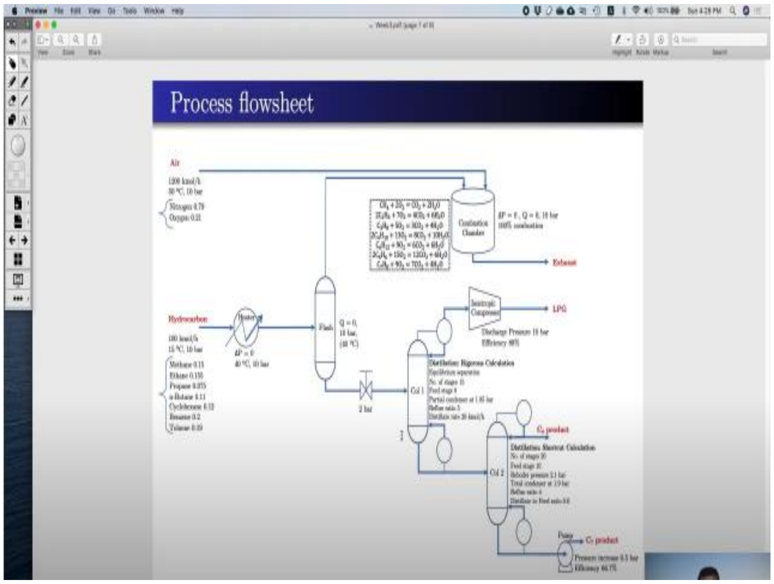

For that we go back to our flow sheet and we find an isentropic compressor whose discharge pressure at this end should be 10 bar and it will operate at 88% efficiency. So, we go back and click on this compressor.

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What is the model and type? So, model it will be compression of turbine and type it will be isentropic. And here we can give various outlet specifications such as discharge pressure, pressure increase, pressure ratio, power required etcetera. So, our specification is discharge pressure which is 10 bar. So, we give 10 bars here. So essentially now although this is complete but some extra information is given here, 88% efficiency.

So, although it is complete, we can give extra information here of 88% efficiency. So, we write 0.88. It is isentropic efficiency. If you do not give any information over here it will take 100% efficiency. So, it will be compressed up to 10 bars. So that is the job of a compressor. Now again we perform the simulation with next button. Well, we must specify the distillation column specification.

So, what are the specifications that we have? Distillation that will be a rigorous calculation. So, it will be equilibrium separation. So, we keep it equilibrium. There will be 15 stages. So, we write here 15 and the condenser will be a partial condenser that is 1.95. Now it is partial vapour because a partial condenser may produce either vapour or vapour liquid both. So, in our case we have only vapour.

We do not have any liquid distillate. So, it is partial vapour. We do not have anything on this side. So, it is partial vapour and then we have some more information. The partial condenser will operate at 1.95 bar. So, that we will see here, yes, operating specification it is still red. So, this two information; we must give. Reflux ratio we must use 5. So, we write 5 over here and the distillate rate here it is 20 kmoles/hr. So, it is 20 kmoles/hr.

So instead of distillate rate you can give bottom rate, reflux rate, boil up ratio, all these things, display to feed ratio, condenser duty. But we have the information distillate rate. So, either of them if you give the equation will be complete. So, its configuration is complete. Let us go to next. So, it is stream. So, it is asking for feed stream. So, where the feed stream is fed? So, we have the information it is 8th feed stage 8.

So, we write it here 8 and then the next one pressure. Pressure condenser pressure which is 1.95 bar. So, we give 1.95 bar then it is also complete. Now here there are certain optional terms. You can check. I mean stage two, pressure or pressure drop in the rest of the column. So, these are the information that you could give but even without them the equations are complete. So, we go to next and here it says run the simulation now.

So that simulation environment is complete with all the specifications written. So, run the simulation now. It simulates with no warnings and no errors and let us check the results. Here see the results. We have a molar flow rate of 20 kmoles/hr. That is exactly what we wanted. We wanted 20 kmoles/hr distillate rate which exactly it is. But we are interested to know what is the composition of LPG?

So, we go here again and check the individual composition. See what are the compositions? Go to mole fraction. So, you see methane is 0.0495, so it is 4.95. Ethane is 23%. It is 0.2298, so it is 23% ethane. 21.78% propane, 45% in butane. And you can see the percentage of cyclohexane, benzene and toluene. Toluene is in trace amounts. Not much of toluene is there but cyclohexane and benzene some percentages they are very small. So that is the specification of LPG.

So, we write here, we rename this thing as LPG. Now we must do something with this flow. It will go to column 2 and this column 2 is not a rigorous calculation. We will do some shortcut calculations. So here go back to the column. We would not use red frag. We will use distill. So, in these distill we will use shortcut distillation using the Edmister method. So, we will bring it over here. So, we go here, reconnect distillation at this point.

And there will be two material balances, two materials out streams and here we will give a total condenser. So, this end will be pumped. So, we need you can see this end will be pumped. So, this is the C7 product, toluene product. So, we go to the pressure changer. We bring in the pump model over here and go to reconnect distillation and connect with this. So, the pump is connected. Go to the material once again, bring it outside. So, this is our C7 product.

So, we rename this with C6 product and this one is C7 product. So, this is C6 and this is C7. Now we can go to the next. It will ask for the specifications of this shortcut distillation and let us rename this B6 column. We have not done it. Neither did we do it for the rigorous one. So, we rename it as say shortcut distill measure. So, this is our shortcut distillation method and this one we write as rigorous distillation.

So, it will ask for the specification of this distillation column and this pump. So, let us press next. It is asking for pump. It could ask for the distillation also but distillation as it starts with s, so it comes later. Pump comes first, p comes first. So, it is asking for pump specifications. So, let us see pump pressure increase is 0.5 bar and efficiency are 66.7%. So, discharge pressure well it does not have discharge pressure.

It says increase in pressure, so it will be pressure increase. We write it 0.5 bar. Now this much is sufficient but still we can give the efficiency of the pump which is 66.7%. So, it is 0.667. Let us press next. Now the distillation column the specification we must give. Now it is a number of stages. It is 20, stage and the feed stage as 10. So, it is 20, feed stage is 10, reflux ratio is 4, distillate to feed mole ratio is 0.6 and condenser type is total.

The condenser pressure again is 1.9 bar, reboiler pressure is 2.1 bar. So, it is condenser pressure 1.9 and reboiler pressure 2.1 and this is a very well-known fact that the reboiler will always be at higher pressure than the condenser. So, our specifications are done. So, it is ready to run the simulation. Again, there is no error and warning. We can now check the output, what is the specification of C7 product? So, we can double click. This is the result.

So, you see here the molar flow is 29.66. We are interested to know about the mole fraction so that we can understand the composition of the C6 product. Here you see methane and ethane 0, completely nothing is there. Propane you can call it zero as well so as butane. These things are not there at all. Cyclohexane is 37.36% and benzene is 62.54%. So, these only constitute the C6 product.

So, you can understand how it is because your cyclohexane it is C_6H_{12} and benzene is C_6H_6. So that is how you have your C6 product. Now along with that you can check the C7 product also because you have already run the simulation for the pump as well. Here you see benzene is only 2.13%, cyclohexane is 2.34%, toluene is 95.48 all others are 0. The lighter key components are all 0. So, toluene is 95.48%.

So, it is mainly C7 products. So, till now we were discussing about the liquid side of the flash tank. Now we are yet to do with the lightest keys that are methane, ethane, and all. So, these things are regarded as the lighter component.

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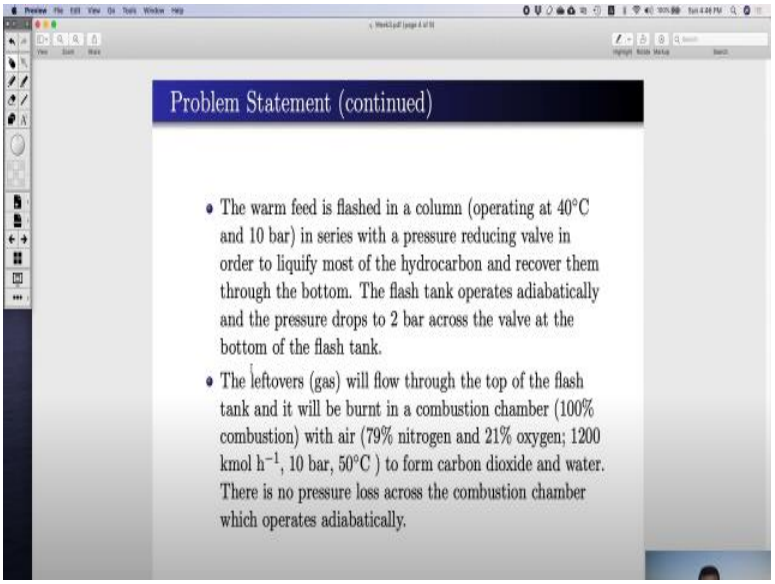

We called it the leftover gas. So, this leftover gas should be burned in a combustion chamber. So, this is a reactor.

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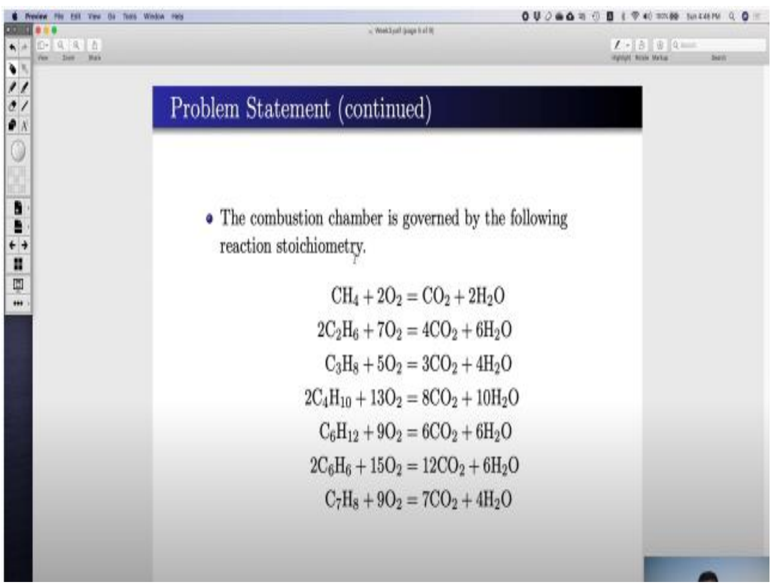

And we know that this combustion chamber will be governed by the reaction stoichiometry. So, we will have a reactor model that runs on stoichiometric.

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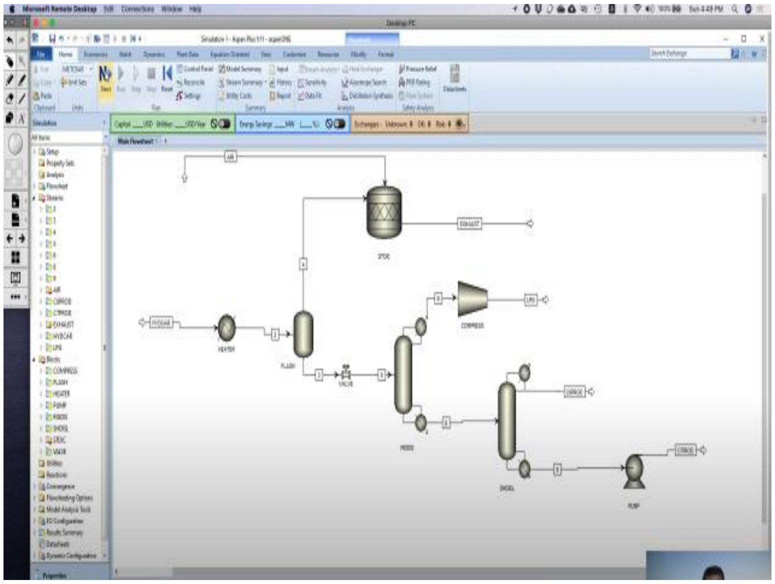

So, for that we must bring in the reactor. So, there are several reactors yield, stoichiometric, equilibrium, Gibbs free energy, CSTR, plug flow, batch. We will use the stoichiometric reactor. So, bring in the stoichiometric reactor over here. We give a name stoic, keep it here and this leftover gas should be sent to this reactor. Now this stoichiometric reactor is not complete without the air because it is used for burning the fuel. So, we bring in a material which is feed.

This is not a very good way of presenting. Although there is nothing wrong in it but we have to make it a bit better so that anybody can understand. Now this is okay. So, this is basically air. The outlet is this one. This is an outlet which will go to sorry this is an extra one we have to delete. Now we must rename it. Let us rename exhaust. So, this is our exhaust gas. Now it will ask for the specifications. Let us press next. Let us see what it asks.

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Now it is asking the air input. What is the input specification for air? Now we are stuck with something new because air does not contain either of them. Air contains nitrogen and oxygen and the exhaust will be mainly CO_2 and H_2O. But we did not do it. We did not include these as a component over there. So, we must include these components as well. So, what we should do? We should go back to the property database. Here we must add a few properties.

So we go to component specification once again. Here we write oxygen. It is so conventional if you write O_2 it will take oxygen over here. Similarly, nitrogen it will take and then CO_2 carbon dioxide, H_2O water. So, all four things which are not there we have brought in. So again, we have to run this next so that the binary interactions again can be calculated along with the new components that we have done. We can safely go back to simulation now.

Yes, now you can see the extra components have been added. Now as we know that air contains nitrogen and oxygen 79 and 21%, so nitrogen will be 0.79 mole fraction and oxygen will be 0.21 mole fraction which will add up to one mole temperature. Its temperature is 50 degree centigrade and the pressure is 10 bar again and molar flow rate is 1200. So, this is mixed. Fine, now we have to go to the stoichiometric reactor.

There let us see what the information's are available. It is a 100% combustion with pressure drop 0, heat duty 0, that is adiabatic, and the pressure is 10 bar. So how we can use this information? Now it does not talk about the temperature. Temperature it does not talk about, but it necessarily talks about the heat duty which is 0 and the pressure is 10 bar. So, either you can write 10 or 0. If you write 0 then it will be regarded as pressure drop and if you write 10 then it will be regarded as 10 bar pressure. Now specifications are there.

We go to the next reactions. Here you must add the reaction components. These reactions you must add in. I will tell you how? You must first set new. Now what are the reactants? The first reaction is methane and oxygen that will react to produce carbon dioxide and water. So, this is carbon dioxide and water. Now coefficient 1 mole of methane reacts with 2 moles of oxygen to produce one mole carbon dioxide and 2 mole water.

And fractional conversion that is component of CH_4 methane is 1 because it is 100% conversion. It is 100% conversion. So, each and every one fractional conversion if it is saying 60% conversion then you must write 0.6 of methane. So, we write next. Now it is showing it is complete because it really does not know whether there is any more reaction going on. So, it is showing reaction complete, but you must give all the other 6 reactions which are written over here.

You must add in all the reactions to make it complete. Now one thing is very common for all the reactions that one of the reactants there is oxygen is common for all of them and the products are also common for all of them. So instead of writing all the equations individually we can copy and then paste it 7 times. So, this is our reaction 1. Reaction 2 it is not methane it is ethane, let us say ethane.

Reaction 3 will be propane, reaction 4 will be butane, reaction 5 will be cyclohexane, reaction 6 benzene and reaction 7 toluene. So, all of them we have given over here. So, each and every one of them we must edit individually. So, this is ethane 2, 7, 4, 6, component ethane. Reaction 2, reaction 1 is methane, reaction 3 propane. So, propane it will have 1, 5, 3, 4. So 1, 5, 3 and 4 fractional propane. Reaction 4 for cyclohexene sorry n-butane 213, 810.

Reaction 5 cyclohexane 1, 9, 6, 6 component of cyclohexane, number 6 benzene 2, 15, 12, 6 and the last reaction is for toluene 1, 9, 7, 4. Now all the reactions are given with their stoichiometry. Now everything is complete. Now next let us run the simulation. Yes, so it is generating the result, no warning, no error. Let us see the result. Exhaust gas we are interested to know the composition of this gas.

So, its molar flow is 1, 2, 4, 2, 6, 6. Mole fraction now we can see it is 100% conversion. So, no methane, no ethane, no propane, no n-butane, no cyclohexane, benzene, etcetera mostly carbon dioxide and water. So, it has 4.54% carbon dioxide, water is 6.86%. Unreacted oxygen 12.29 and the nitrogen mole fraction is 76.28%. So, nitrogen is there without any reaction. If you see the mass fraction or mass flow rate, the role of nitrogen you will see.

Here you see nitrogen 26556.8 kg/hr. Compare it with the original air. What did you send? You send the same amount of nitrogen. So, nitrogen remains unreacted, it is an inert component. But oxygen you send 8000 kg/hr and unreacted is 4889.77 kg/hr. Rest of the oxygen has reacted and, in the air, there was no carbon dioxide and water. But in the exhaust, you find 2487.7 kg/hr of carbon dioxide that is produced out of the stoichiometric reaction. So, this is the complete simulation of the process flow sheet that we have discussed so far.

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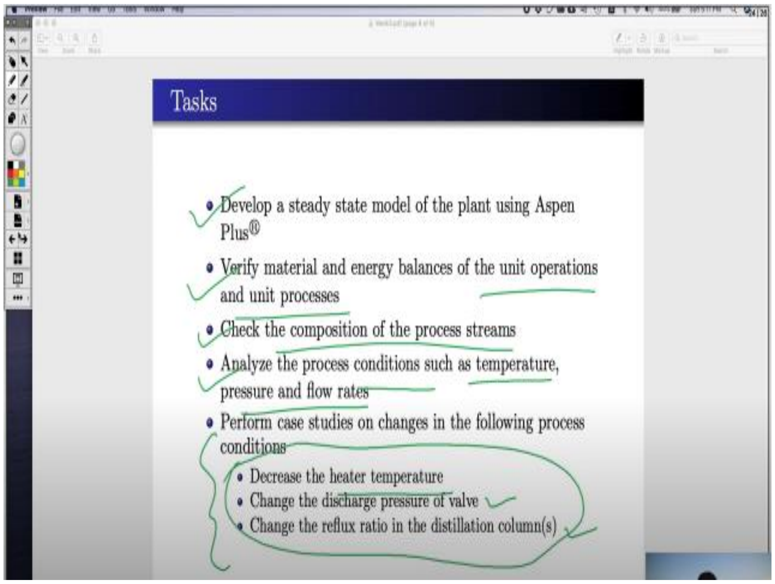

Now we have developed a steady state model of the plant. We have verified the material energy balance of the unit operational unit processes. We have checked the composition of the process streams. We have analyzed the process conditions such as temperature, pressure, and flow rates and now we are left out with doing this stuff that is perform case studies on changes in the following process condition. First, we will decrease the heater temperature and see what happens.

Then we will change the discharge pressure of the valve and, we will change the reflux ratio in the distillation column and see what happens in these three cases. So, let us first go now here let us here the temperature was 40 degree centigrade. Let us decrease it to 30 degree centigrade and see what happens. So please note that here the temperature earlier it was 40 degree centigrade and now it is 30 degree centigrade.

Now, it will affect the flash condition and because here there is heat duty 0. So, whatever the heat that is coming from here it will be going through these two streams. Now let us see whether there is any change that happens with these.

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So, the result in the number 4 we had mole flow of 30.5667. So, it is 30.5667. So much of the mole of leftover gas is going upwards. Now if we run this simulation from 40 to 30 let us see what happens. Remember earlier it was 30.5667. Now the simulation is run. Now let us check what is the result. So here the result is 28.2006. Earlier it was 30.5 something now it is 28.2. So, it necessarily means that if your heater temperature is down then the less amount of material will be vaporized.

So, the per hour mole content of the leftover gas will also reduce to some quantity. Earlier it was 30 point something now it is 28 point something. So, this is the effect of reduction of heater temperature. Now let us go back to our old thing that is 40 degree centigrade and rerun the simulation and check our calculation. It should again come back to 30. Yes, now it is 30.5667. Now then we must change the discharge pressure of the valve.

Now let us go to our second one that is the change in discharge pressure of the valve. So the discharge pressure of the valve right now is 2 bar. And the outlet the stream 5 its composition results in molar liquid fraction is 88.1031%. So, if it is compressed to 2 bar it is 88.10%. Now if the valve pressure is increased to 5 bar then obviously the liquid percentage should increase. Let us see whether it happens that way. So, remember it is 88.10% for 2 bar pressure.

Now let us say it is 5 bar and for 5 bar it should increase from 88.88% to something. Let us see whether it increases and to what extent it increases. So now we go back and check the valve 5 results. Here you see the molar fraction is now 95%. So, it increases from 88% to 95% by changing the valve outlet pressure from 2 bar to 5 bar. Now let us see what the effect of change in reflux ratio is. Now before that let us do one more thing.

Let us change the valve pressure to say 1 bar that is atmospheric pressure. Let us see what happens here. You may expect some interesting results. That means we are saying that we will change the valve position in such a way that this stream will have 1 bar atmospheric pressure. Now let us run the simulation. And here we have got the first warning of our simulation. Please note the warning. This is the first warning for the simulation.

Let us examine why we are getting this warning. Here we are having 1 bar pressure. What is the condenser pressure of this? Check the condenser pressure is 1.95 bar. So essentially, we are saying that our feed pressure is 1 bar and condenser pressure is 1.95 bar which cannot happen. I mean until and unless we use some kind of pump or something it cannot happen that way. Aspen is doing the calculation as per the information it is given to it, but it is giving you the warning also that unless you fix this warning your design may be wrong.

So, we go back to 2 bar pressure and run the simulation. Now we shall see our last task that is change in reflux ratio in the distillation column. So, let us check the distillation column say take this distillation column. Here our reflux ratio is 5. And suppose we reduce the reflux ratio to 3. So, if your reflux ratio is decreased, quality composition should be decreased. But if we need to keep the distillate composition intact then we need to increase the molar enthalpy of the reboiler. So that is the logical conclusion.

Now the reboiler output results what is the molar enthalpy? It is 358 calories per mole. So this much enthalpy is needed or if we decrease the reflux ratio to 3 then the logical conclusion is the molar enthalpy of this stream should increase. So, this one should increase to 358.3 should go higher. Let us see whether it happens and if it happens then to what extent. So, we run simulation now.

Now it becomes 364. From 358 to 364, so molar enthalpy increased. So, the opposite thing will happen if the molar enthalpy is sorry the distillate, the reflux ratio is increased. So, the opposite thing happens with instead of 5 if it is 7 then if we run it and check stream number 7 results from 358 it decreases to 354. This is what is expected. So, if we increase the reflux ratio then the molar enthalpy of bottom flow rate will decrease.

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So, this is the conclusion of our small exercise on hydrocarbon treatment. So, we have developed the model of hydrocarbon treatment method in the Aspen simulation domain and we have run the simulation. We have analyzed the results and we have done a few case studies on that. Thank you.