Aspen Plus Simulation Software - A Basic Course for Beginners

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Lecture - 01
Significance of software with example – Simulation on Pen and Paper vs. Simulation on Aspen Plus

Welcome to the massive open online course on Aspen Plus. This course will enable one to learn the use of Aspen Plus software for process calculation, process engineering calculation, modelling, and simulation. Before going into the details of this course, let us go through a short preamble that will enable us to understand what is process modelling and simulation in general and how Aspen Plus can be used for this purpose?

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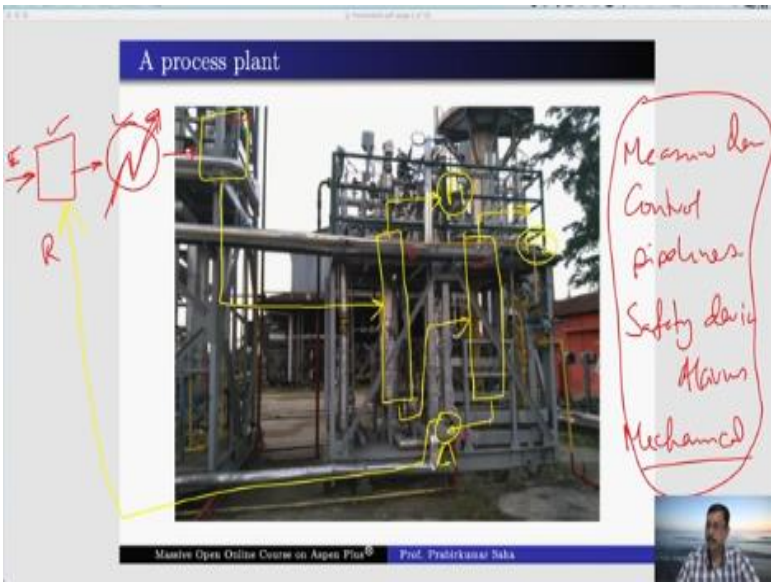

Let us consider this process plant. Now, this is not actually a full-fledged plant; rather, it is a small unit of a large plant. Now I will explain the individual equipment that is present over here. The main equipment in this unit is one distillation column; there is another distillation column over here, there is a pump, there is a small reactor, and there is also a heater, and there is a mixer. So process feed is passed through this heater and the mixer in series before it is fed into the reactor.

The reactor output is then fed into the distillation column. Here the distillate is the product of this unit P1, and the bottom stream of the distillation column 1 is fed into the second distillation column

where the distillate is product number two of this unit. The bottom stream of the distillation column is then pumped back to the mixer. It is a recycling stream. So basically, the mixer mixes the fresh fit and the recycle stream, and the mixture is then fed into the heater to get heated up, and it is sent to the reactor.

Now, in addition to this main equipment, there is plenty of other ancillary equipment and devices such as measuring devices, control system units, there are various pipelines, there are safety devices, and alarms, and there are mechanical structures as well, which are necessary to build these processes units. Now, for the time being, these are not important for the focus of our discussion. We pick and choose only these six units for our discussion because these are the principal units.

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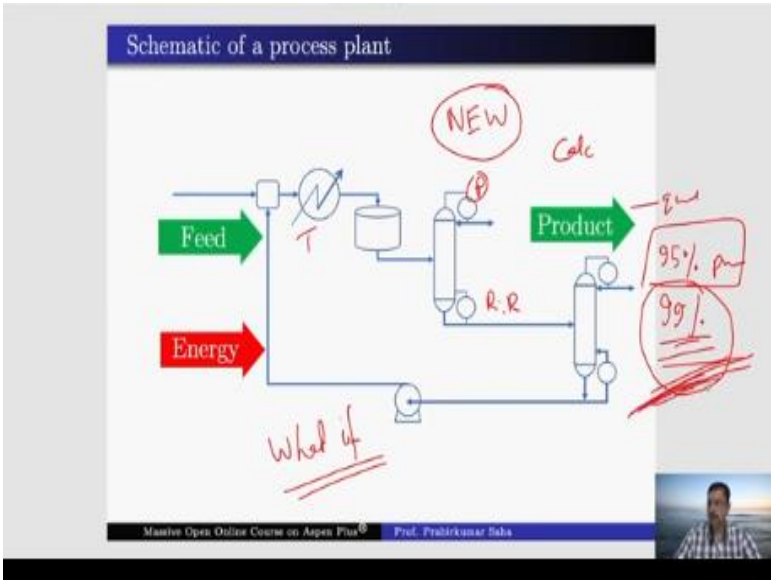

Now we make a schematic of the process plant where we have kept the principal units that are the mixer, the heater, the reactor, distillation unit 1, distillation unit 2, and the pump. These six units we have kept. All other things we are not interested in. Now, what happens in this unit of the process plant? We give feed. Feed means the material feed. The feed which is being heated up before it goes to the reactor, and the reaction happens. The reactor content is then distilled.

That is the feed, material feed, and also we have energy feed. Because we have to operate the heater, we have to operate the condensers and the reboilers of the distillation column. We have to operate the pump; we need electrical energy. So basically, in this process plant, we have to give

two types of feed. One is material feed, another is energy feed, and the product we will get out of it this is P1, and this is P2, two types of products.

So ideally we have to make sure that these products they are up to the desired standard of their quality and quantity. In other words, we have to make sure that the product rate, the flow rate of the product, and its quality is maintained. Now whatever we have in the process plant, what could be the major tasks of a process engineer out of it? What may be the duties? The first one we may have to design a new plant. This plant may not be in an existing condition.

As a process engineer we may have to design it for some purpose, and that design can be given to the fabricator for fabrication and then installation. In order to do that, we have to do certain calculations based on some mathematical calculations, or we may have to work with an existing plant of this nature which is there for years together. It might have served us for several years before the market demand has changed the scenario. In the market nowadays, the product quality may be different in demand. So we have to change the product quality.

Earlier say 95% purity might be enough. But nowadays our competitor is selling at the same price and 99% purity. Obviously then our product will not be sold in the market. In such a situation, we have to revamp our process to meet the market demand. So we have to change a few things. We do not know what to change, but we have to do some what-if analysis. That means if we change the heater temperature if we change the condenser pressure, if we change the reboiler ratio, how far the product quality will change?

So these are the various what-if analyses that we can do in order to arrive at the market demand quality. Now, these things cannot be done in the real-life plant. The plant manager will not allow one to go and middle with the system. So one needs to do on pen and paper some calculation. How to do that calculation?

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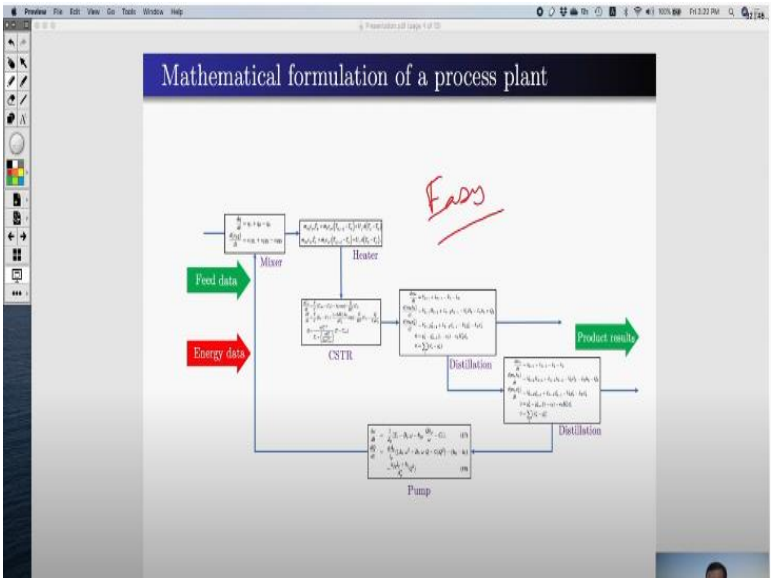

We all know we have to replace these processes or we have to replace this equipment with their mathematical counterpart. Here you see we have replaced the mixer, heater, CSTR. All of them have been replaced by a set of differential and algebraic equations, and these equations have been taken from the textbook. They are well-known equations. They have been developed from mass balance, energy balance, rate equations for CSTR, the vapour-liquid equilibrium in case of displacement column, etcetera.

So these are all standard equations whose structures are the same. No matter which distillation column you use, they remain the same. What changes? The number of trace change in a distillation column, the components change. In one distillation column, you may work with methanol, another distillation column, you can work with ethanol, and so on. So based on the component that you use, your property database will change, the flow rate, temperature, pressure, those things will change.

But the structure of the equation remains the same. So if your structures are the same, you need to feed the data. When you work with mathematical formulation, the real-life feed is not of any use. Here you have to use the data. If it is flow rate, then you have to give some information about how many kilo moles per hour or how many Kg/hour or what is the quality, whether 50 mol % or 25 wt.%, etcetera.

And also energy data in terms of joule or for a continuous system it is wattage joules per second. So these data have to be fed into the process, and the calculations can be done. All these equations have to be solved simultaneously, and you know how to solve simultaneous equations. For example, if you have an equation:

$$3x + 2y = 5$$

you cannot solve this equation because you have two unknowns and one equation. So you have degrees of freedom 1.

There may be plenty of solutions with pairs x and y. But you have to fix either of them; then the other things will be fixed. But instead, if you have another equation like

$$5x + 9y = 11$$

then obviously you have two equations and two unknowns. You have degrees of freedom zero that means there will be only one pair of x and y. For this, the system is defined. So the same idea has to be reflected with the entire plant.

Here you have to count the number of equations in these units, and you have to see how many variables you have accordingly. You have to fix some of the variables as per your requirement and the process data then they are mostly temperatures, pressures, and inlet conditions, etc., and when the degrees of freedom is zero, it is ready to run the simulation. So all the equations run parallel, and then the output result comes out of the calculation. Now, this kind of operation 50 years back people used to do on pen and paper because they did not have any other option.

But nowadays, after the advent of computers, people write computer code because that is easier for calculation. But for a complicated system, even writing computer code is also tedious. For example, a distillation column each and every tray they have at least three ordinary differential equations. One is for mass balance, one is for component balance, and the third one is for enthalpy balance.

And this balance occurs at each and every tray. Suppose a distillation column has 50 trays, then we have to solve 150 parallel ordinary differential equations. Now talk about two distillation columns; the number rises to 300 and add on the equations of pumps, CSTR, heater; it will be a

gigantic task. Now the question is there any other option for easy handling of these equations? The answer is Yes; Aspen Plus does it. How?

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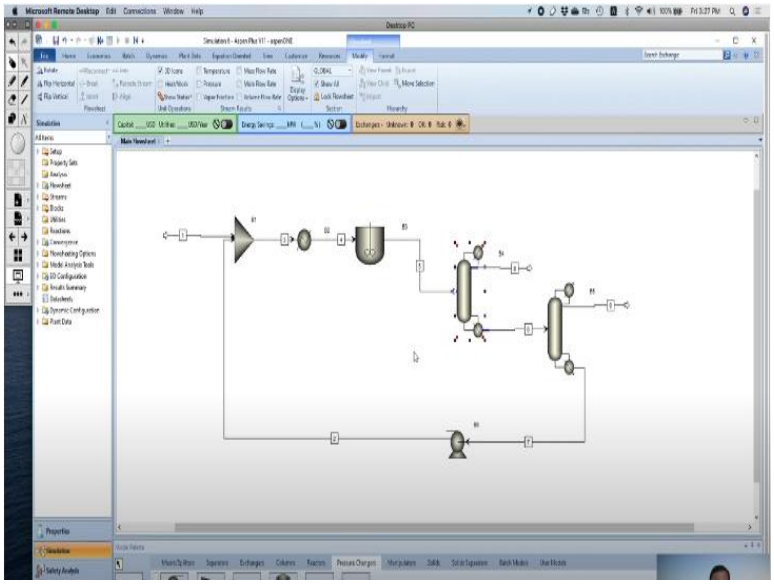

You take the example of this. This is the Aspen Plus window. We will go into the details of the window later. We will learn it later in detail. But I will show how it is done. At the bottom, you can see the model palette. Here you have the models of mixer, models of separator, models of heat exchanger, column, reactor, pressure changer, and so on. So what you can do if you want a mixer you can simply drag this over here.

If you need a heater, just go to the exchanger bring it over here. If you want the reactor, just go there, and CSTR brings it here. Similarly, bring the columns, distillation column, another distillation column, and lastly, we need a pump. So bring the pump over there, and these are the six units you need, and now we have to connect the material stream. So the red things are required; without them, nothing can happen in the simulation.

So it requires one or more material streams. So this is the fresh feed. It is connected with the extensive product. So this is connected to the pump output and the recycle loop they are mixed. So mixer output is connected to the heater, the heater output is connected to the reactor, reactor output is connected to the column, first column output is connected to the second column, the second column output is again connected to the pump.

And we have here product 1 and here product 2. Now here, you can see the same structure, the model, the unit we have connected. Now each and every module, this is only the front end. The actual calculation happens in the background. So when we are dragging the column, all the equations associated with the column they are taken into the simulation in the background. We do not see these equations. But those equations are there behind them at the backstage.

In the front end, we have a small icon that represents the distillation column. Now, as you understand, in the distillation column, you have to set some values. Just look at the values what we need to give?

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We need to give the number of stages, we need to give the feed stage we need to give the reflux ratio and so on. So these are the data we have to feed in. But the background equations we do not bother because they are all set by Aspen Plus. We do not have to pick and choose those equations. So this is how the entire operation works in Aspen Plus. So this is menu driven. It is a designer's delight.

One designer can always add in this diagram, and a designer can always add in certain new equipment. He can just disconnect it. Suppose if I want to disconnect, then I have to put right-click, and then we can cut. Then this vanishes off. This also we can cut, and this vanishes off. Instead, we can use some other column. We can use a rat frag column which is also a distillation column. We can put in here, and then we can connect or reconnect the stream at the destination over here.

And then again, we can reconnect this stream with the source which is here, and finally, this is our product. So when we delete something, then all the equations associated with that particular module it also vanishes, and when we add in something, then all the equations associated with them they come in. So that is the beauty of Aspen Plus's front end. So this is the flowsheet model. We will learn it later in detail.

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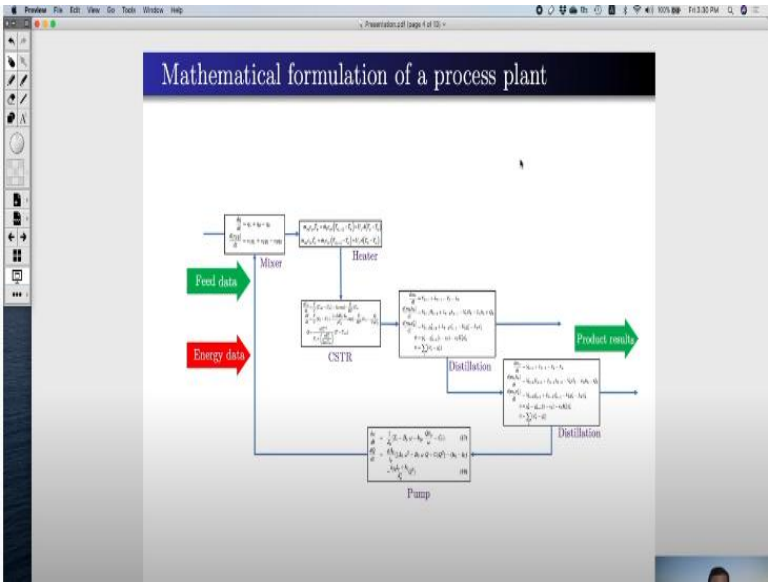

So this is how the mathematical formulation can be done.

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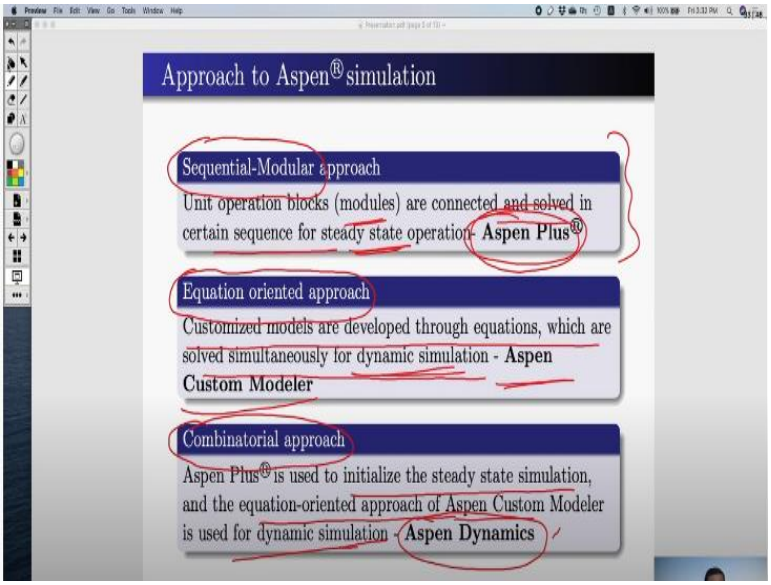

So we talk about the approach to Aspen simulation now. Just now, whatever we had discussed that is actually a sequential modular approach. That means we take some module and that we place them in sequence and then those unit operation blocks they are called modules. They are connected and solved in a certain sequence for steady-state operation. This is called Aspen Plus. But not all the unit operations that are available in chemical engineering or process engineering unit they may be standard.

Like the distillation column is standard, reactor is standard, heat exchanger is standard. But there is some equipment which may be non-standard equipment. So you will not find a standardized model in the model palette. For them, you have to write your own customized equation in order to work with. So you have the next one equation-oriented approach. There you have to work with customized models those are developed through equations that are solved simultaneously for dynamic simulation.

Here it was the steady state, here it is dynamic simulation, and this is called Aspen Custom Modeler. And lastly, there is a combinatorial approach where Aspen Plus is used to initialize the steady-state simulation, and the equation-oriented approach of Aspen Custom Modeler is used for dynamic simulation, which is Aspen Dynamics. Now in this particular course, we have only Aspen Plus. We will discuss Aspen Plus. For Aspen Custom Modeler and Aspen Dynamics, there may be someone who may float a different course altogether. So we will limit ourselves with Aspen Plus.

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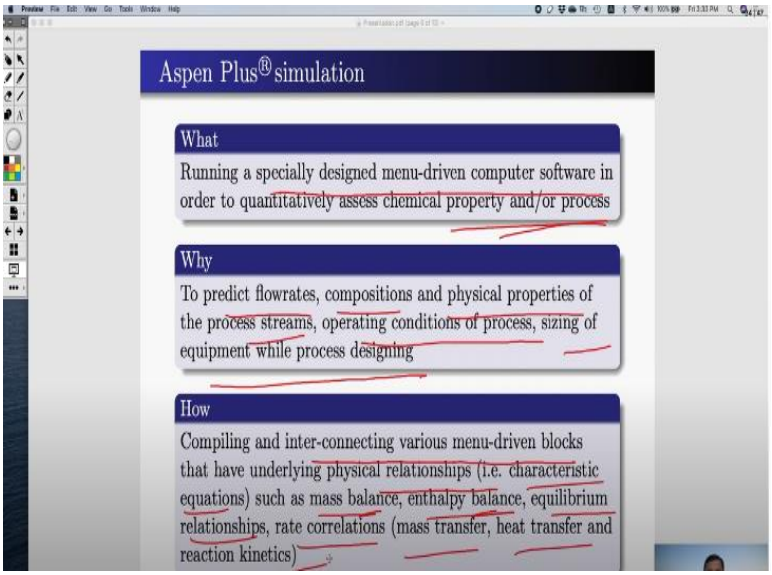

So we summarize what we learn in the Aspen Plus simulation. What is Aspen Plus simulation? It is about running a specially designed menu-driven computer software in order to quantitatively assess chemical property or the process. Why do we do it? Because we want to predict the; flow rate, the composition and physical properties of process streams, operating condition of the process, sizing of equipment while process designing, etcetera.

And finally, how do we do it? We do it by compiling and interconnecting various menu-driven blocks that have underlying physical relationships that is characteristic equations such as mass balance, enthalpy balance, equilibrium relationship, rate correlation like mass transfer, heat transfer, and reaction kinetics.

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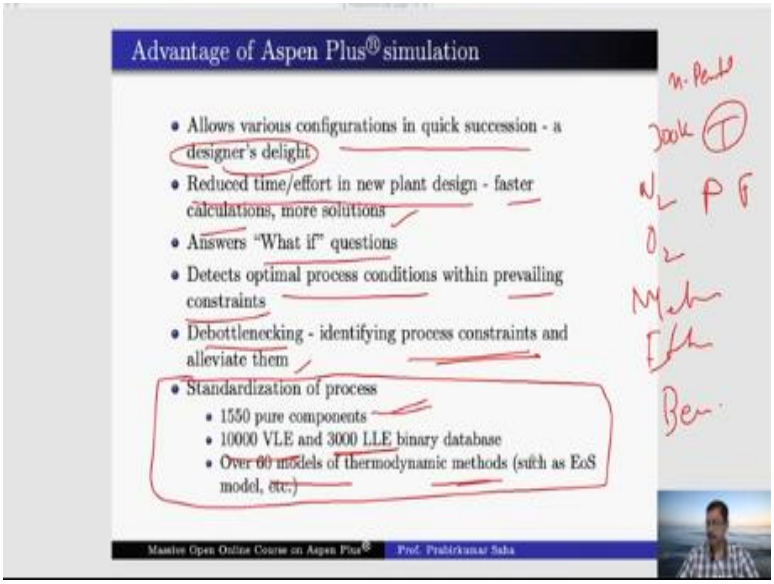

And these are the advantages of Aspen Plus simulation. It allows various configurations in quick succession, which is a designer's delight. Just a few minutes back I explained how the blocks can be taken out of the flowsheet and how a new block can be inserted. So the person, the designer does not have to pick and choose the equations out of his or her computer code. He has to just delete certain models or add certain models and everything is menu-driven.

So it can be done very quickly, and the simulation also can be done very quickly. As a result, we will have reduced time and effort for new plant design because you can do faster calculations. You will have more number of solutions to analyse and arrive at the appropriate design calculations. And it answers what-if questions that we have already discussed, and it detects optimal process conditions within the prevailing constraints.

Sometimes the hard constraint comes, like suppose the calculation it arrives at a 110% valve opening, but in real life, 110% valve opening is not possible. The valve can open only up to 100%, not more than that. But in real-life calculations, when we want to do some optimization, these

kinds of constraints will come into the picture, and we have to work with them. So debottlenecking that means identifying those process constraints and alleviate them. That is also possible with Aspen Plus.

And last but not the least this standardization of process is very important. All the common process engineering unit operations are modelled, and they are standardized and not only the model along with the data. Data for nearly over 1500 pure components like if you want to use some common components like nitrogen, oxygen or some hydrocarbons like methanol, ethanol or benzene you do not have to look for their data. The Aspen has options; you can pick the component from its database and attach them.

Aspen Plus knows where to bring the data from at what temperature. So you just fix the temperature and pressure, and flow rate. Suppose we want to find out the specific heat, which depends only on the temperature. So we have to say the component in pentane at temperature say 300 kelvins. Aspen will bring the data from its data bank. We do not need to look for the data for that. So it has pure component data; it has over 10 000 Vapour Liquid Equilibrium (VLE) databases.

Also it has 3000 Liquid Liquid Equilibrium (LLE) binary database and it has over 60 models of thermodynamics methods like the equation of state. We can talk, we can use Peng-Robinson method, Readily Quanks Wave method etcetera. Those who are very conversant with thermodynamic methods, you know what I am talking about. So these are the advantages of Aspen Plus.

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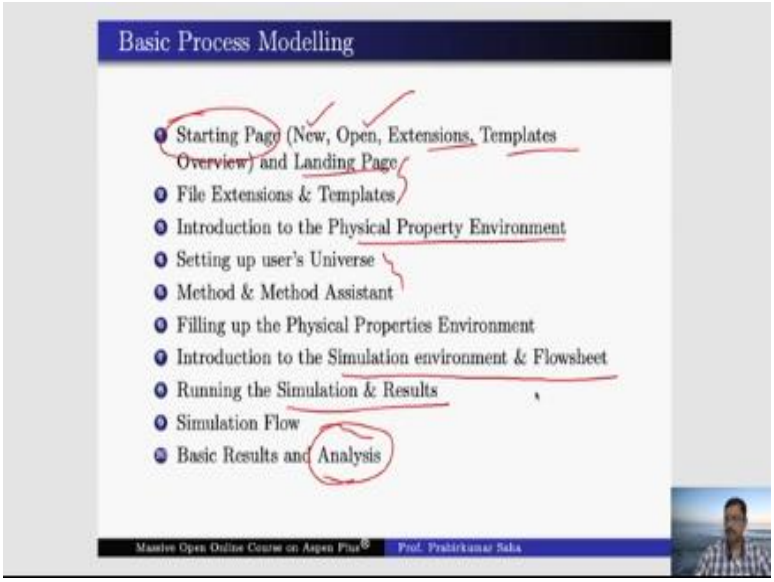

Now to work with Aspen Plus, first, we have to understand these basic process modeling features. So we will begin our Aspen Plus training with basic process modeling. We will learn what is the starting page. We have already seen a glimpse of the starting page a few minutes back. We know what is how we will learn how to open a new simulation box, how to open an existing one, what are the extensions, templates, overview?

We will be introduced to the physical property environment setting up the users in inter-universe method and method assistant, then we will be introduced to simulation environment and flowsheet. Again we have seen a few glimpses, then we will learn how to simulate and get the result, and finally, we will see how to analyse the result.

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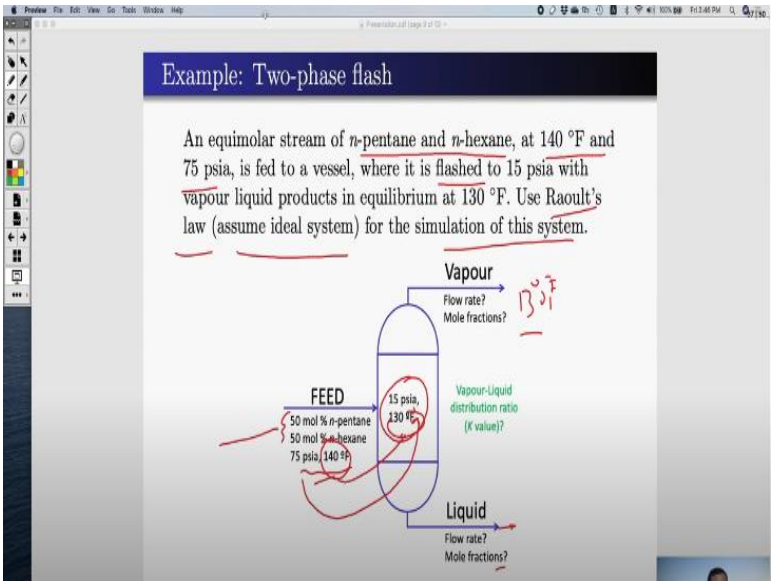

Now the best way to learn a software is to watch someone using this software, and a better way of learning it is to go through a simple example. Now we talk about a two-phase flash which is the simplest example that I could think of. Now first, we will learn what is the problem and then we shall solve the problem in a textbook approach. We will take the theory from the textbook data also from Perry's handbook.

And solve it on pen and paper, and later we will do the same thing in Aspen Plus, and then we will see how far the data and the results match. So the problem is something like this. An equimolar stream of n-pentane and n-hexane equimolar that means 50-50 mol % at 140 degrees Fahrenheit and 75 psia temperature and pressure is given. It is fed to a vessel where it is flashed to 15 psia with vapour and liquid products in the equilibrium at 130 degrees Fahrenheit.

So you can see both temperature and pressure they are reduced. So the pressure is maintained at 15 psi temperature is also maintained at 130 degrees Fahrenheit. So one thing is sure the feed condition is at 140 degrees Fahrenheit, and the outlet condition is at 130 degrees Fahrenheit. So these are the different temperature conditions that we have. Now, what is to be done? Use Raoult's law. That means it is an ideal system we have to assume for the simulation of this system. That is the job that we have.

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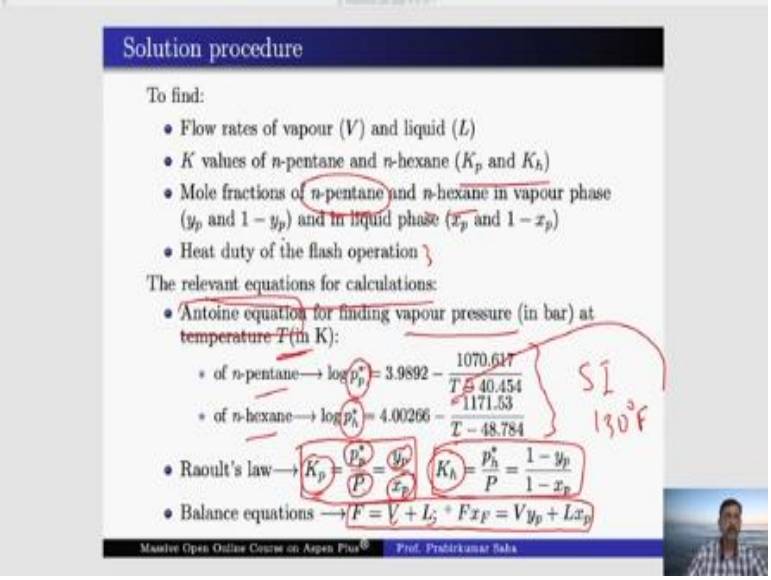

So this is the solution procedure. We have to find flow rates of vapour and liquid. Let us represent it at V and L. The K values of n-pentane and n-hexane, we have to find the mole fractions of n-pentane and n-hexane in the vapour phase and liquid phase. So y_p and x_p are for pentane, p represent pentane. So y_p is for n-pentane, x_p is also for n-pentane in vapour and liquid phases, respectively.

Antoine equation for finding vapour pressure (in bar) at temperature T (in K);

* of *n*-pentane→ $log^*_p = 3.9892 - \frac{1070.617}{T-40.454}$
* of *n*-hexane→ $log^*_h = 4.00266 - \frac{1171.53}{T-48.784}$

And as it is a binary system so 1 minus y_p is n-hexane and 1 minus x_p is n-hexane in vapour and liquid phases. And lastly, we have to calculate the heat duty of the flash operation. Now, these are the relevant equations for calculation. The first thing we have to find the vapour pressure, and we know the Antoine equation is used for finding the vapour pressure and vapour pressure depends upon the temperature. And here, we have two equations rather for n-pentane and n-hexane.

These are the vapour pressures of pentane and hexane at this temperature. Now we have to use Raoult's law. So what is Raoult's law? This is Raoult's law where

$$K_p = \frac{P_p^*}{P} = \frac{y_p}{x_p}\ ,\ K_h = \frac{P_h^*}{P} = \frac{1 - y_p}{1 - x_p}$$

Where,

Vapour pressure (P^*_p)

Total pressure (P)

mole fraction in vapour phase (y_p)

mole fraction in liquid phase (x_p)

So this is for pentane (K_p), and this is for hexane (K_h). So we know P if we can calculate we know the temperature 130 degrees Fahrenheit equivalent in kelvin we have to calculate.

So we can understand how to calculate them. So if we know vapour pressure and total pressure is known we can calculate K_p and K_h. So if we know K_p and K_h then we have two equations and two unknowns. So we can easily calculate x_p and y_p. So if we know x_p and y_p the lastly the balance equation we know everything in these equations except V and L which can be found out very easily and next is the heat duty calculation.

- Balance equation$\rightarrow F = V + L\,;\, Fx_F = Vy_p + Lx_p$

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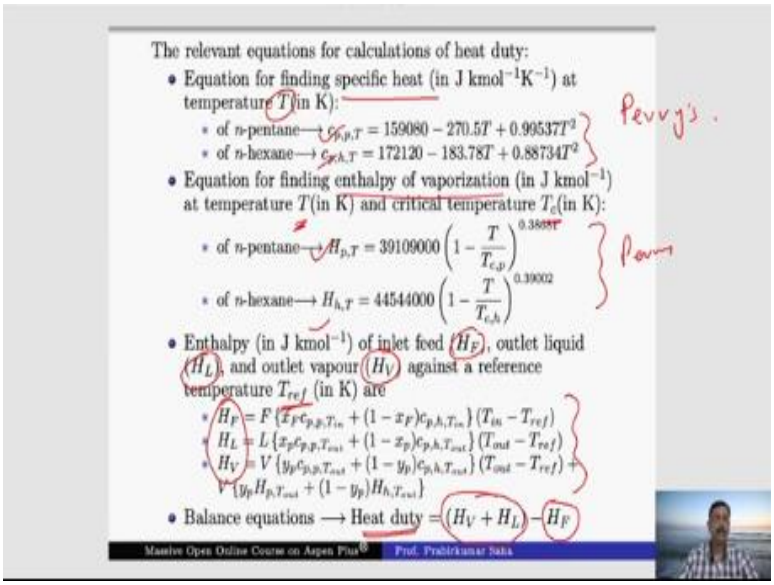

For heat duty, the relevant equations are you have to first find out the specific heat. This is the specific heat at temperature T. Specific heat is also a temperature-dependent function, and these are taken from Perry's handbook. Similarly, equation for finding enthalpy of vaporization at

temperature T and at critical temperature T_c these are also taken from Perry's. We can calculate all these four.

- Equation for finding out specific heat (in J $kmol^{-1}K^{-1}$) at temperature T (in K):
    - of n-pentane$\rightarrow c_{p,p,T} = 159080 - 270.5T + 0.99537T^2$
    - of n-hexane$\rightarrow c_{p,h,T} = 172120 - 183.78T + 0.88734T^2$
- Equation for finding enthalpy of vaporization (in J $kmol^{-1}$) at temperature T (in K) and critical temperature T_c (in K):
    - of n-pentane$\rightarrow H_{p,T} = 39109000\left(1 - \frac{T}{T_{c,p}}\right)^{0.38681}$
    - of n-hexane$\rightarrow H_{h,T} = 44544000\left(1 - \frac{T}{T_{c,h}}\right)^{0.39002}$

So enthalpy of inlet feed outlet liquid and outlet vapour against a reference temperature because we know the enthalpies are always calculated against a certain reference temperature. So these are the equations for calculating H_F, H_L and H_V, and we all know about this value. Nothing is unknown. So we can calculate them. So heat duty will be the heat out minus the heat in, the enthalpy out minus enthalpy in, so that is the heat duty.

- Enthalpy (in J $kmol^{-1}$) of inlet feed (H_F), outlet liquid (H_L), and outlet vapour (H_V) against a reference temperature T_{ref} (in K) are
    - $H_F = F\{(x_F c_{p,p,T_{in}} + (1 - x_F)c_{p,h,T_{in}}\}(T_{in} - T_{ref})$
    - $H_L = L\{(x_p c_{p,p,T_{out}} + (1 - x_p)c_{p,h,T_{out}}\}(T_{out} - T_{ref})$
    - $H_V = V\{(y_p c_{p,p,T_{out}} + (1 - y_p)c_{p,h,T_{out}}\}(T_{out} - T_{ref}) + V\{y_p H_{p,Tout} + (1 - y_p)H_{h,T_{out}}\}$
- Balance equation$\rightarrow$ Heat duty $= (H_y + H_L) - H_F$

So, that much heat has to be fed to the flash tank. That is the hint. So this is how we calculate. The calculation procedure is like that. So these are the calculations.

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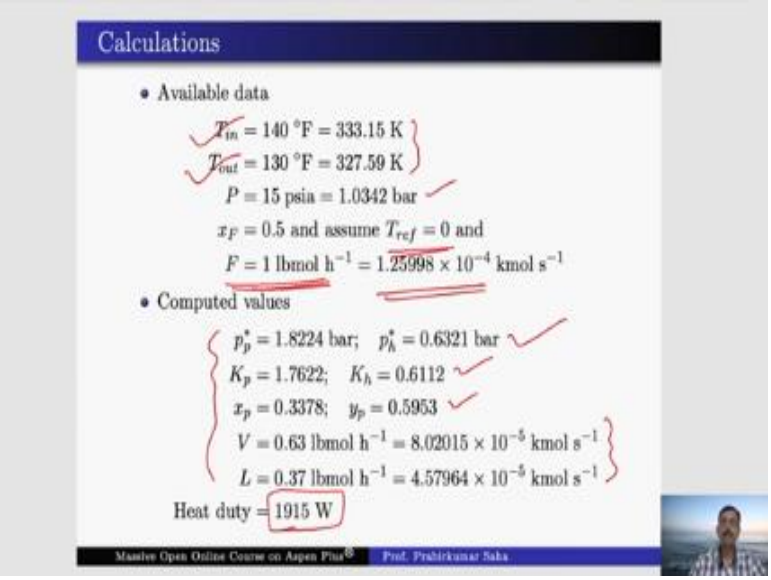

We have the available data T_{in}, T_{out} they have been converted into the SI unit so as pressure P. Now we have to assume two things one is reference temperature. We can take anything. I have taken zero. It does not matter because in heat duty calculation if you heat duty calculation it is the difference in enthalpy. So reference temperature should be same for all the enthalpy calculation and the feed basically in a continuous system everything is calculated per mole basis.

So just for the calculation's sake, we have to take a number. So we have taken one-pound mole per hour, which actually is in terms of kilo mole per second. It stands to be like this, and these are the computed values based on them. We have calculated the vapour pressures to be like this. On that basis, we have calculated the K values. On that basis we have calculated x_p and y_p. On that basis we have calculated V and L, and finally we have found the heat duty to be 1915 Watt. Now let us do the same calculation in Aspen Plus.

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First, we have to fix the components. Now we have two components over here. One is n-pentane; another is n-hexane. So we do not know where to find the n-pentane and n-hexane. So we take the help of this button. Just increase a bit and here we write pentane and find. Here Aspen Plus will dig out all the components that have remote connection with the word pentane. So just see we have 1, 1, 2 trimethyl cyclopentane, 1, 1, 3 trimethyl cyclopentane and so on. Here we have 1, chloropentane. So from this list, we have to dig out the one which we are looking for. This is the

one that we were looking for. So just press add selected compounds. Here this is added N PEN 01. It has given a component id which anyway we can change any time, and this is the component name C5H12 is the alias. Similarly, we can go for a new search, say hexane. Here again, we have to dig out the component.

Yes, this is the one that we are looking for and now we can close it. So these are the two components that we have got n-pentane and n-hexane. We can change it anytime. Suppose we are not happy with this component id n pen. So we write pentane and here we can write hexane. So instead of pentane and hexane you can give any name. It does not matter. It is just an id. This is the next. I mean, for any Aspen Plus, for that matter, for any simulation, it is always best to go to the next button.

Next button it says that go to the next input sheet needing input. So many times, we do not know where to go, but the next button, if you press the simulation, will take you the point where the next input is required. Now it is asking for the method base method. That is the property method. Now we know that we have to work with Raoult's law which is an ideal system. So our base method is an ideal system.

So it is ideal property method uses both Raoult's law and Henry's law just in place. Now you can see here there is an icon which is half red and half white. This means that the input is incomplete. The moment input is complete; you will find a blue tick like this. So the moment I choose an ideal you see a blue tick that means the input is complete here, until unless the input is complete you cannot find this blue tick here. Now our property input is complete now we have to go to the simulation database.

(Video starts: 47:36)
Now in the simulation we have to build the flow sheet first. Now in the flow sheet here we have a single flash tank. So we have to look for flash. It is available at separator. So this is two outlet flash, model flash drums, evaporator etcetera with rigorous vapour liquid or Vapour Liquid Liquid Equilibrium. Now our case matches with that we have two outlet flash with vapour liquid equilibrium. Now we have to add the material stream.

So the red means always it is asking for input. So it is asking for one input and two outputs. So this is the feed. This is the feed input, this is the vapour output and this is the liquid output. We can rename it. So let us rename it as feed. We can rename it as vapour and we can rename it as liquid. Again it is just a simple name it does not have any other significance. Instead of vapour you can write V also instead of liquid you can write L also.

Now again you write you press next it has gone to streams feed input. Now it is asking for input. So what is the feed condition? So as we know the feed condition is 50 mol % n-pentane, 50 mol % n-hexane 75 psia pressure and 140 degree Fahrenheit temperature. So here the inputs are all in SI unit. But our data has been given in British unit. So we change it from metric to English. See it is asking for English unit.

We can mix and match, we can give it in C, we can give it in kelvin also. But whatever we give, the Aspen Plus software has its own way of converting the unit as it demands. So we give the data 140 degree Fahrenheit and 75 psia pressure and then the total mole flow rate we have used one-pound mole per hour. So it is one-pound mole per hour. Now it is still half red and half white because we have not given the composition.

So composition we can give it in mole flow rate or mole fraction, mass fraction, standard volume fraction etcetera. We will give it in mole fraction. So pentane is 50%, which means 0.5 and hexane is again 0.5, so the total is 1. This is the total mole fraction 1. The moment I give 0.5, 0.5, it becomes a blue tick. That means the simulation the input stream specification is complete. Now, this is still the block input block b1, that is, the flash it is asking for input.

We can directly go there, or we can just safely press; next it will come to this one. It is always safer to press next rather than going directly over there. Here again, it is asking for temperature and pressure, which are given. Instead of temperature, one can give heat duty. Temperature fixing; means we have to supply the heat in such a manner that the temperature is fixed at 130 degree Fahrenheit. Now instead, we can say that I will not give more than this much of heat duty.

Let the temperature fix; let the block fix its own temperature. So either you can fix temperature, or you can fix heat duty, not both. In this case, we have to fix our temperature because the problem states like that. So the temperature is how much it is 130 degree Fahrenheit and pressure is 15 psi. The moment I give it is blue ticked. That means all of them now are blue ticked. So the required input is complete. Now we press next; there is no input required.

(Video starts: 54:13)
It is asking to run the simulation now all the required input is complete. You have to say yes, run it. So it is running the simulation in the background. Basically, it is working with all the sets of equations that we have brought in from the model palette to the equation to the flow sheet. Now we go back to the simulation you see what happens. These are the loading simulation engine, processing input specification, flowsheet analysis, competition order for the flow sheet.

Calculation begins for block 1 flash 2 simulation calculation completed. No warning, no error generating result. So we have got some results. So go to the result summary. What are the streams? We have three streams and all these streams are given here. Feed, liquid, and vapour. What is their temperature? See liquid temperature feed is in liquid phase. What it says? The feed at 140 degree Fahrenheit has to be liquid.

Vapour phase, vapour liquid phase, liquid temperature is 140. So both liquid and vapour we have 130 degree Fahrenheit. But feed is 140 degrees, pressure 75, 15, 15. Now, smaller calculations with sub stream mole flow. So how many moles of vapour and liquid we see? 0.63653 lbmol/hr 0.36347 lbmol/hr. Now let us check with our calculation. Just go back here you see we had calculated V = 0.63, it is 0.63653, L = 0.37, here 0.37.

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There will be slight variation in calculation because Aspen may not use the Antoine equation. It has its own data bank which it is using, and what about the mole fraction of pentane? 0.3378 in liquid phase 0.5953 in vapour phase. So it is almost the same mole fraction. You see the mole fraction pentane liquid phase 0.33, vapour phase 0.59, 0.59, 0.33, and lastly, the heat duty. Heat duty we have calculated to be 1915 Watt.

So let us go back to the block b1 here some results are given. Heat duty is 6811 bit is thermal unit per hour. Now if you want to see it in Watt just go there. Watt it is 1996. Our case it was 1915. So 1.9 kilowatt. So it is also 1.9 kilowatt. Now this much of error is evident because we use Antoine's equation, whereas Aspen Plus has its own set of equations and database, which is proprietary in nature. They are very much realistic, and they are tested out.

So that is how we solve it in Aspen Plus and the results are also matching. So instead of going through this tedious calculation, we can simply put it in Aspen and do the calculation in a very simple manner. Now suppose if you want to change something, if you want to change the feed input from, say 75 psi or 140 degrees to 150 degree Fahrenheit then we have to run the simulation once again, and the heat duty will definitely change. Let us see what is the heat duty. Earlier it was 1996 now, it is 18.48.

So the heat duty has reduced. So this calculation is very fast. A design engineer can perform these calculations very fast and very effectively. But the same calculation if you have to do in this fashion then it will take a long time and sometimes very tedious. So that is the advantage of Aspen plus. Now with this small introduction in the next few lectures, we will go into the detail of how the Aspen Plus software can be used most effectively. Thank you.

(Video Ends: 01:00:19)