

Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 43

Solving a Distillation Column Using Aspen Plus

Hello, everyone. In this class, we are going to see some demonstration using a commercial process simulator, particularly Aspen Plus. So, as you know, Aspen Plus is a tool or industry process tool, which helps you to make steady state calculations of different process involving the different physics, whether it is a distillation column, whether it is the reaction system or whether it is coupled system like multiple units are connected together in process.

That how do you solve for those systems and calculate the different stream flow rates and the stream conditions. So, mainly the calculations are done in steady state. There is also recent development where you can do unsteady calculations, but primarily this is for steady state calculations. Most of the thermal dynamic models are actually you know, incorporated into the into the system.

So, you have a large variety of material database, as well as thermodynamic properties. Now, in this class, we will be particularly looking into the simulation of a distillation column using the different algorithms that we have been discussing in the last few days. So, it has different modules or different capabilities in using those particular modules or those particular algorithms that we have discussed.

So, first in this introductory class of Aspen demonstration will try to give you some brief overview of the different components, the different setups or settings, assuming that you are a starter in this, using this software. And in the next couple of classes are essentially the remaining classes of this week. We will also talk about some more example problems with increasing levels of complexity.

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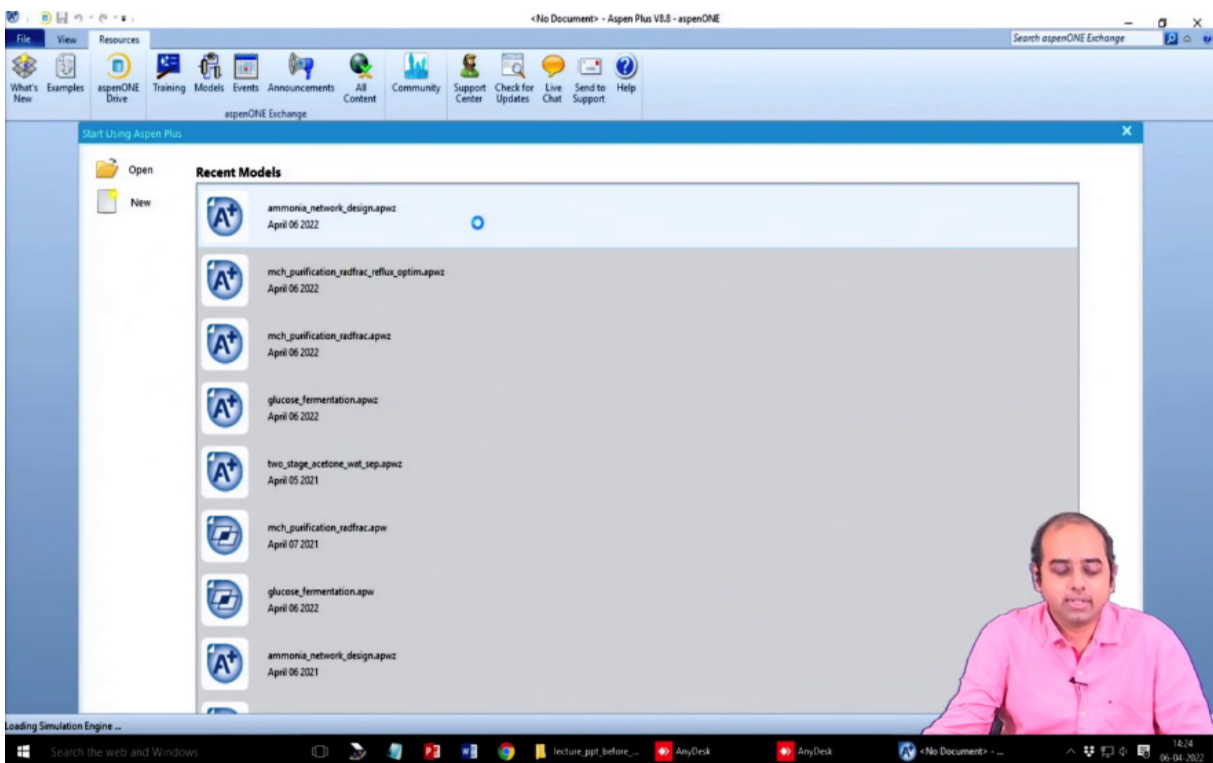
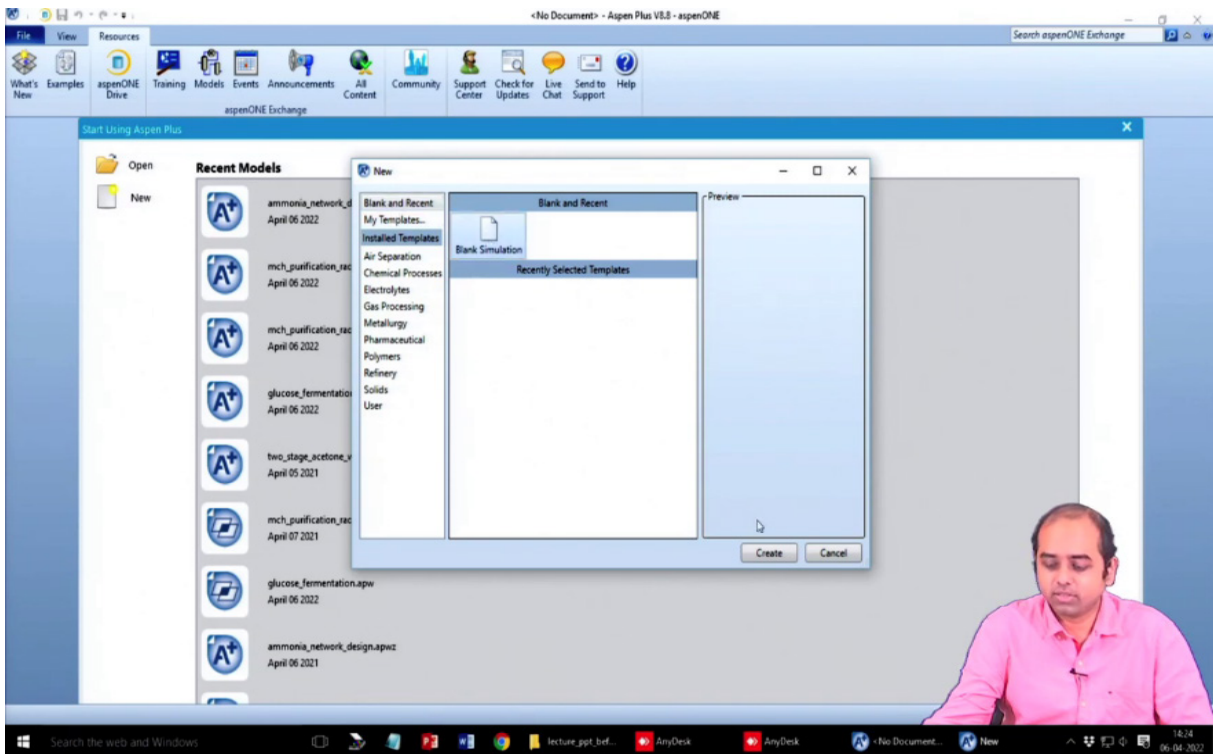
CONCEPTS COVERED

- ❖ Basics of the Aspen Plus software
- ❖ Solving a simple distillation using RadFrac module
- ❖ Sensitivity analysis

NPTEL

So, we will focus particularly on the distillation column or a multi-stage distillation column, try to understand that what are the optimum, these number of stages, finding out the optimum feed stage and then trying to see that how distillation can be enriched, how the distillate can be enriched using this entrainer. So, before we go to the details about the problem, first, let me give you a brief overview of the different components of the software.

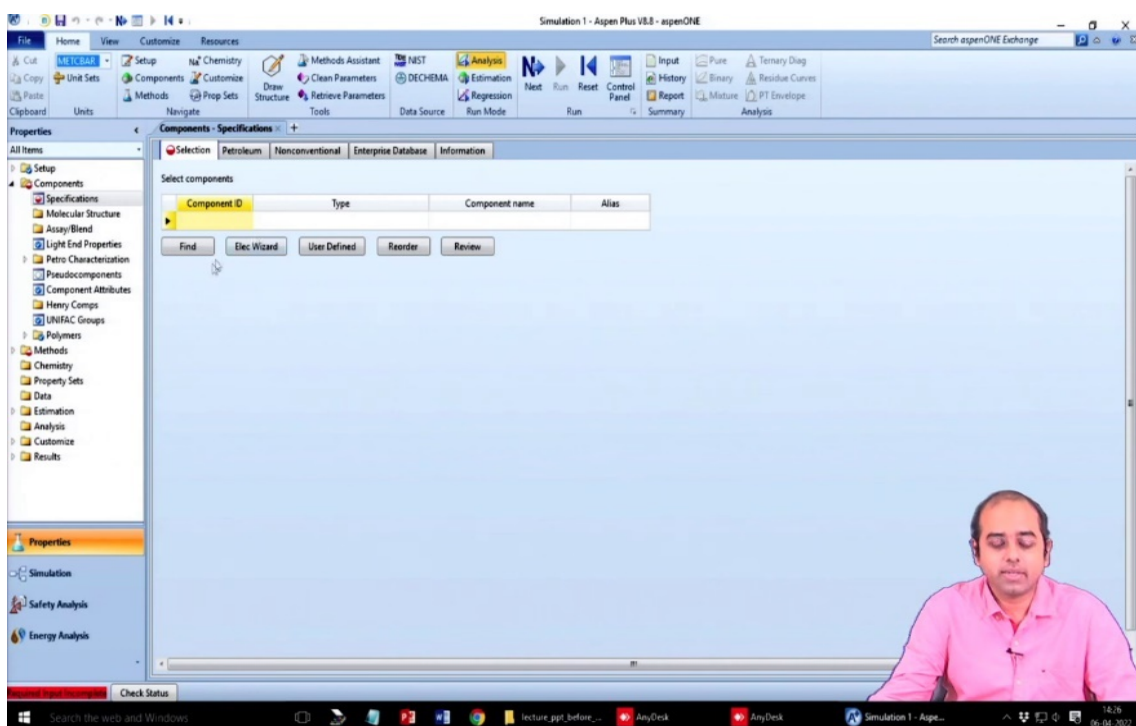
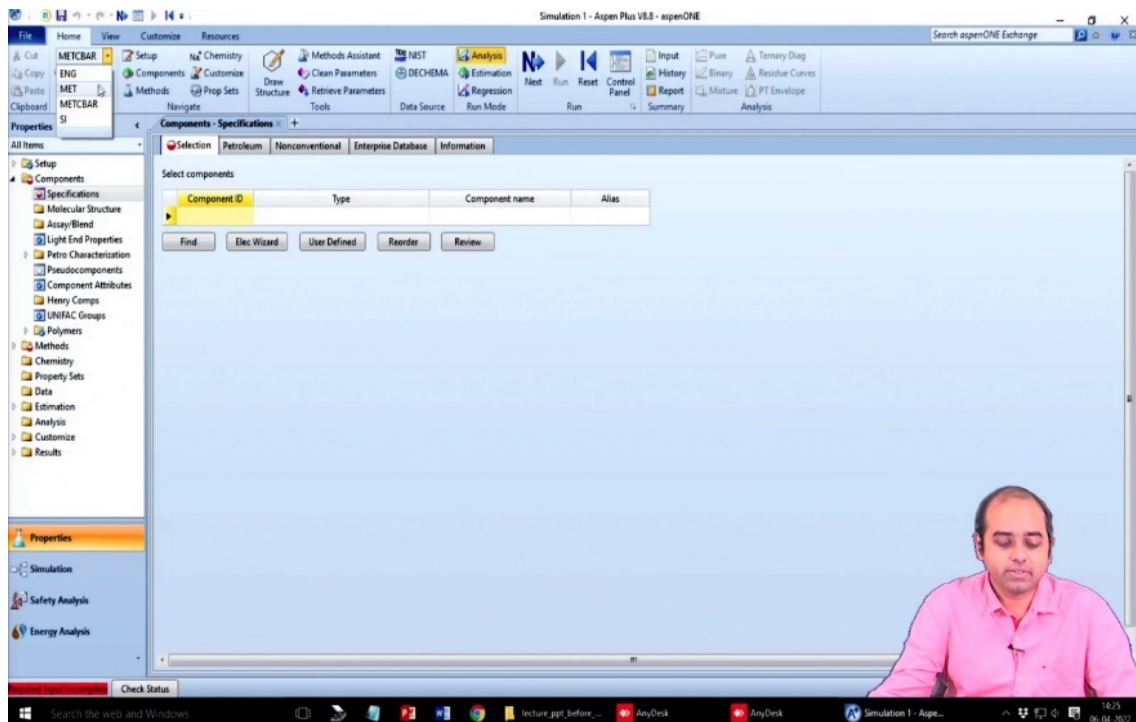
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So, this is Aspen Plus. This is the window of the Aspen Plus software. And as you note that this is a paid license that I am using. So, depending on your situation, either if it is there in the university or you request for a demo license, you can get access to it at least for a trial period. So, this is Aspen Plus version 8.8, and this is a part of the aspenONE Suite. So, there are many other products in aspenONE Suite, for example this pipeline P and ID, construction design, define simulation and et cetera. But this is what we are focusing on Aspen Plus.

So, now in Aspen Plus actually there are two options. I can open an existing file to create a new one. So, let us say, create the new one. And it will ask that what kind of template do you want to select? So, best is to go by blank simulations. I have selected blank and I have clicked on create. So, it will start a blank simulation. And let me show you the different streams present and the different components of the overall layout of the software.

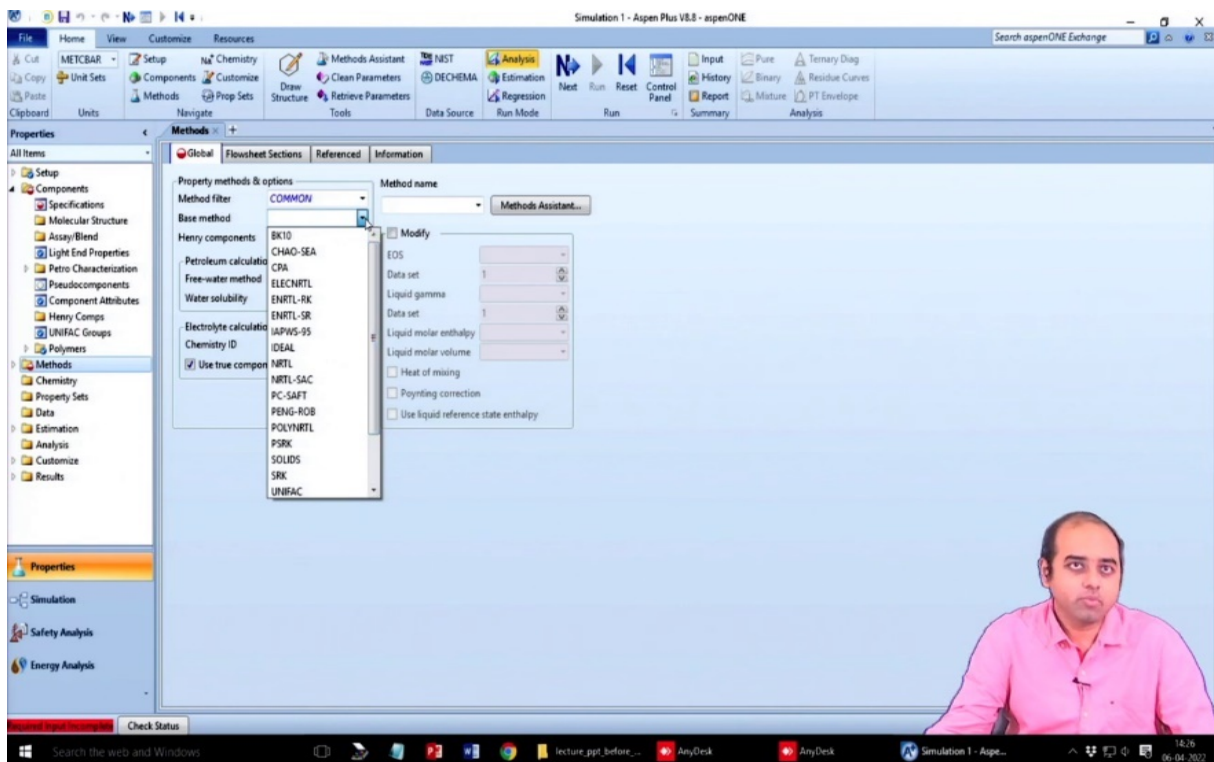
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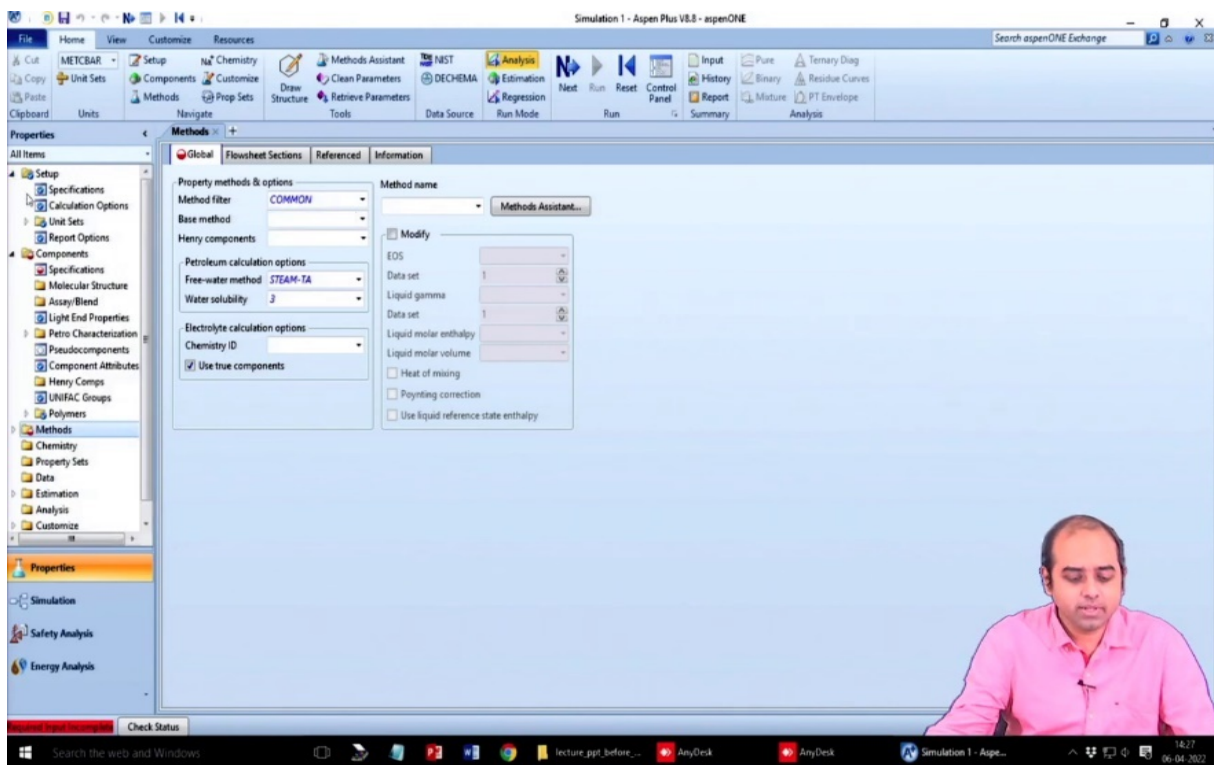
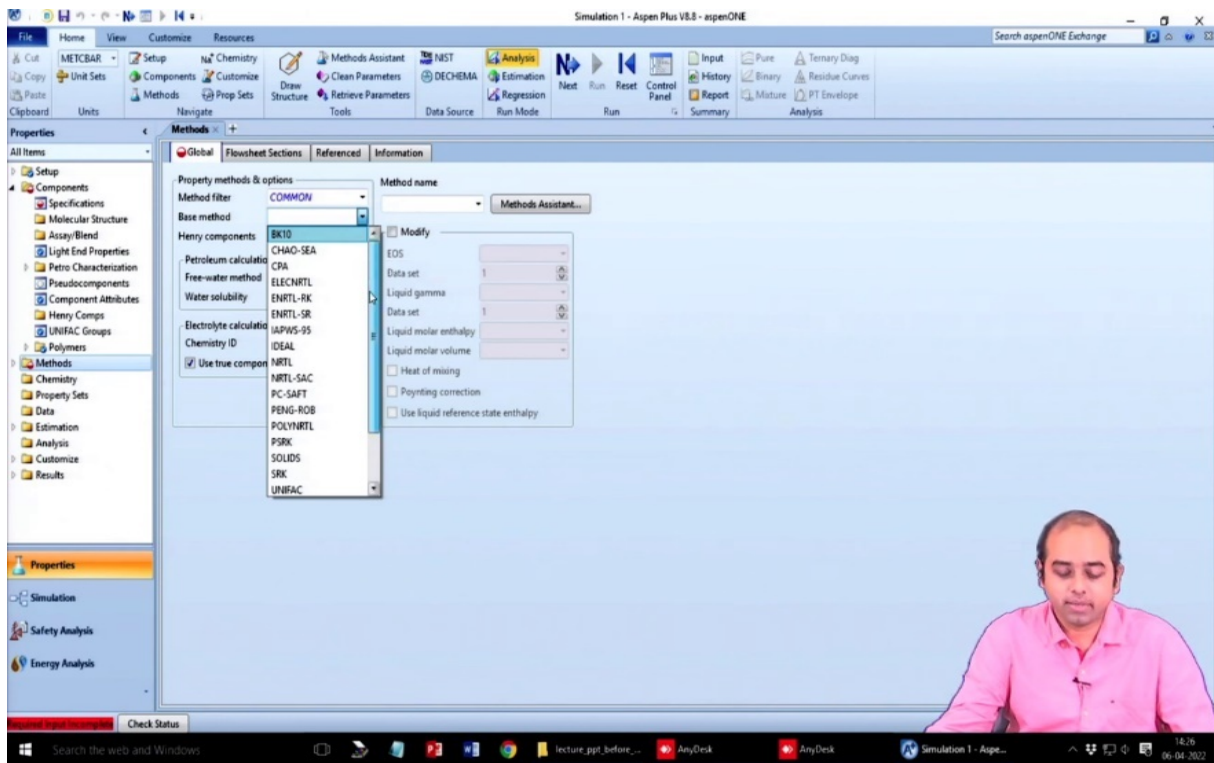


So, just to give you a bird's eye view on the left-hand side, you see that there are four different tabs. The first one is the property, second one is the simulation, third and fourth are energy and safety analysis. So, first, you have to define the property. First, you have to define the property. What are the components that you will be dealing with in this system? So, accordingly it will search for the components from its database, and it will add it to your system. It has quite an exhaustive database.

So, most common chemicals are already present. So, you just have to find out using this wizard and enter those specifications. We will talk about in detail when you look into the problem. Next is the unit. So, what sort of units do you want to select, whether it is an engineering unit, whether it is a metric or SI units, whatever sort of units do you want to select has to be specified first as the top. After selecting the different components or the chemicals.

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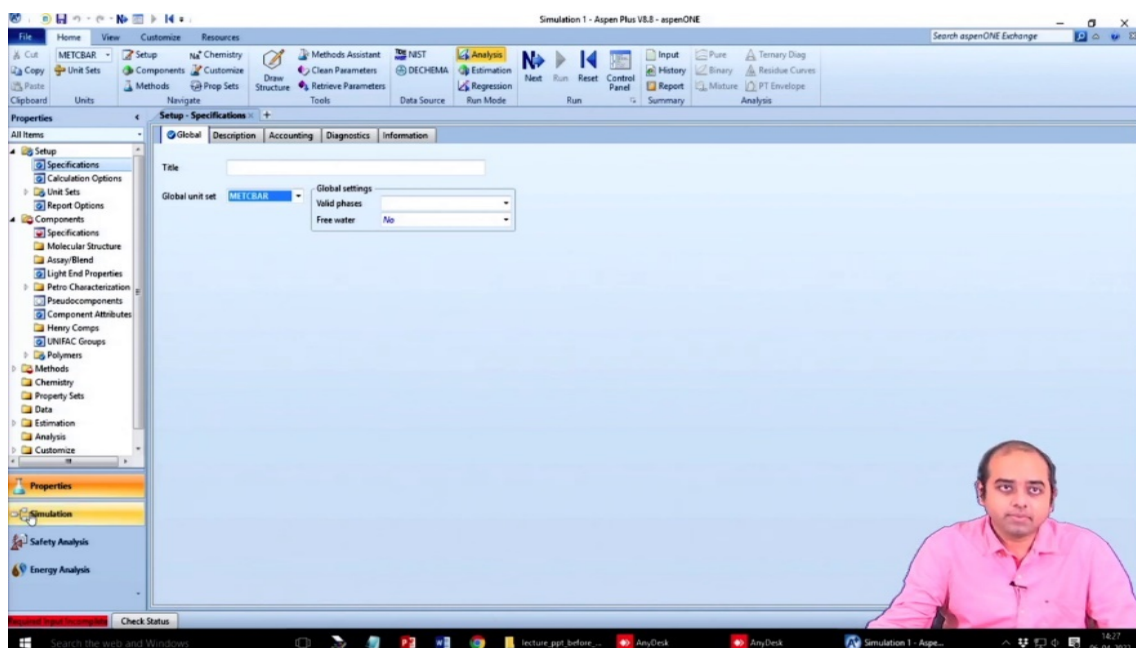
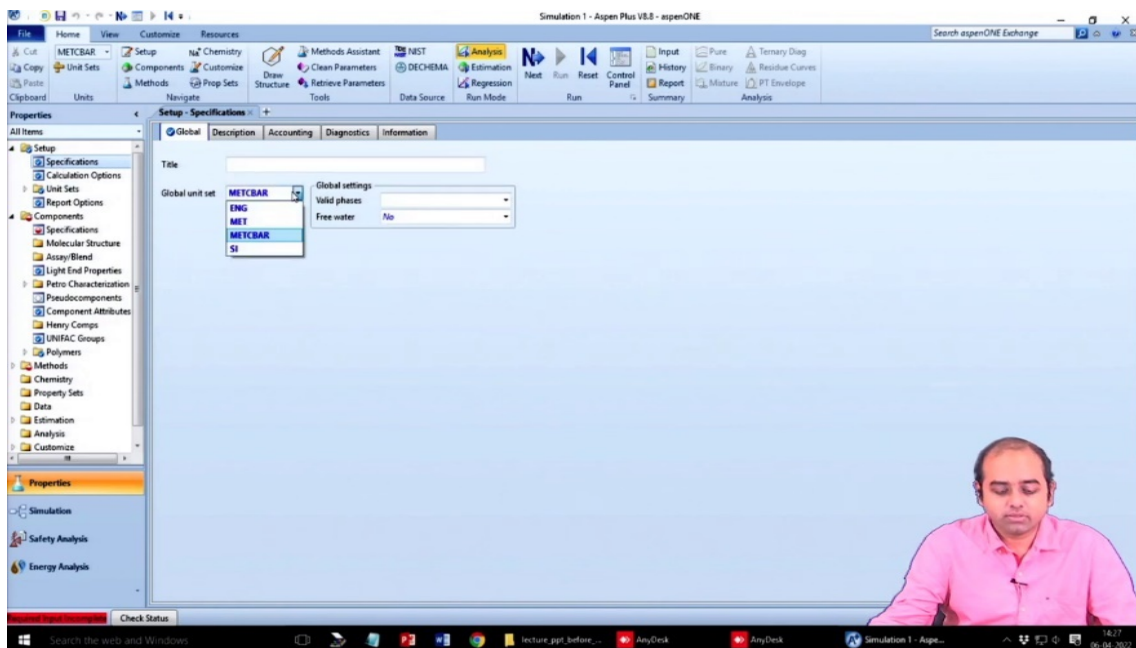


The next thing you need to do is to specify the method. Which thermodynamic models should be used to compute different properties, it is equilibrium values, et cetera. So, if you look into these base methods, these are some of the popular thermodynamic models and many of you must be or I guess all of you have already studied several of these models in your chemical engineer camera dynamics.

And as you go towards the bottom, you will see that some of the more complex models, UNIQUAC and UNIFAC, WILSON, et cetera there. So, the general recommendation is to choose a most comprehensive model maybe UNIQUAC or UNIFAC. Now, once you select these two, there are some more analysis which can be done here.

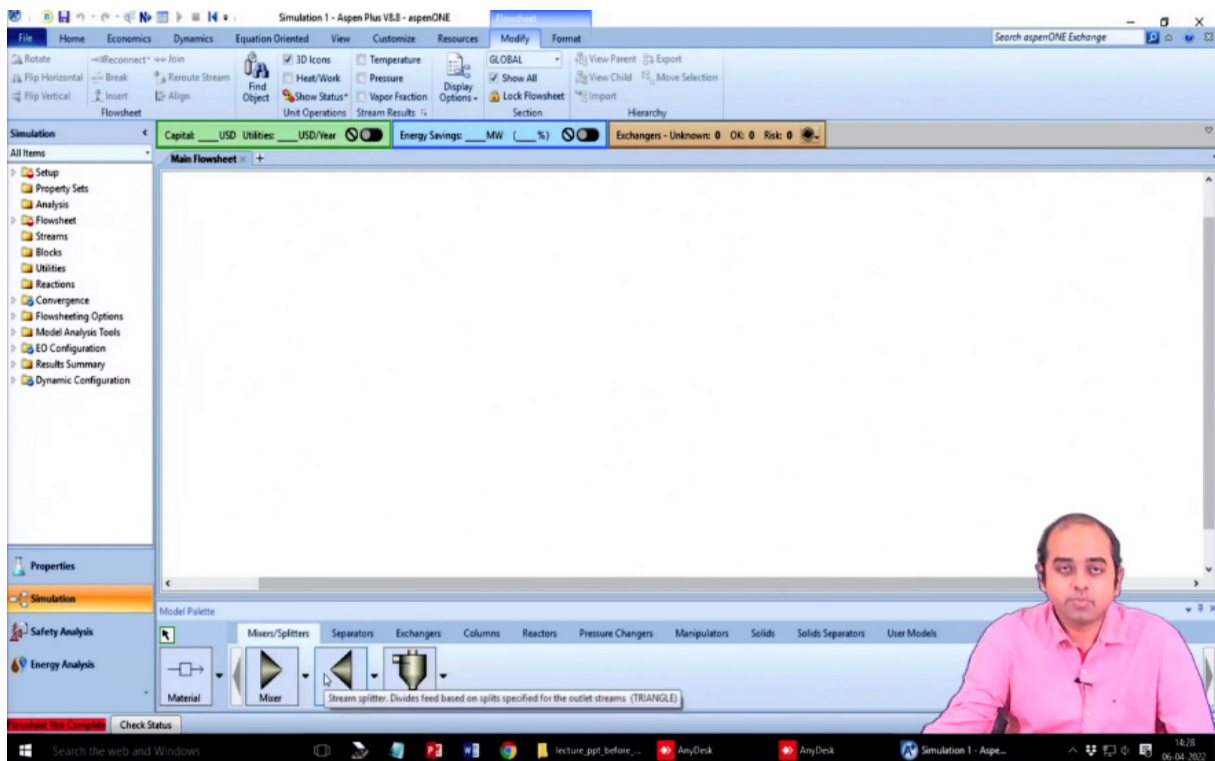
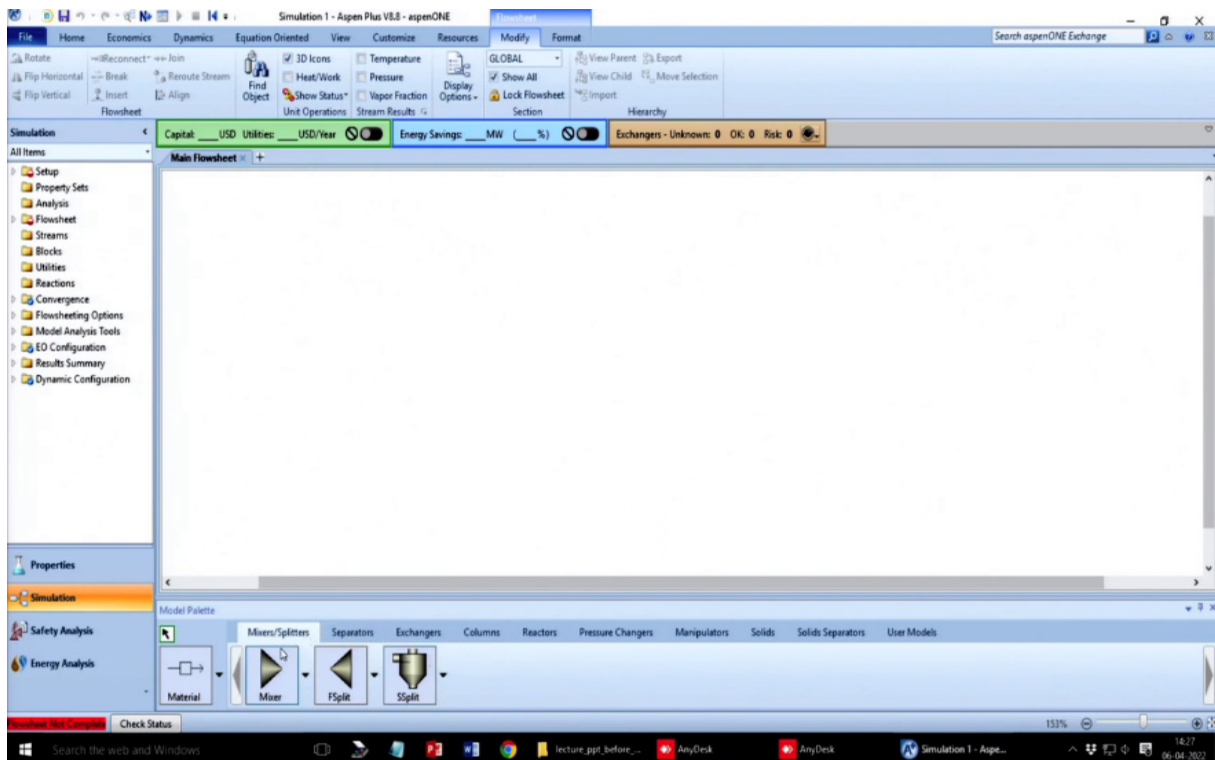
And that is something I will show you later when we do into the problems. Like for example, trying to work out the phase diagram of three components, alternative diagrams of three components from using calculating the values from its property database. So, once these two are set up here, there are some more specifications.

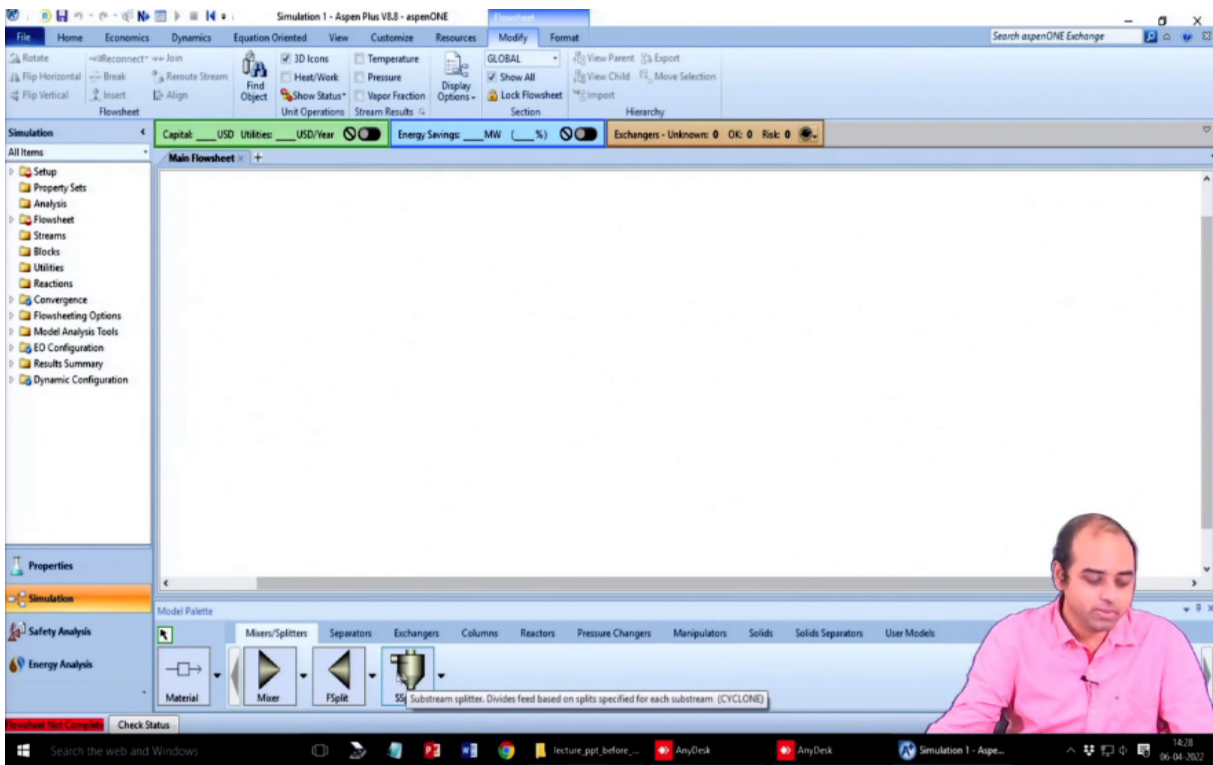
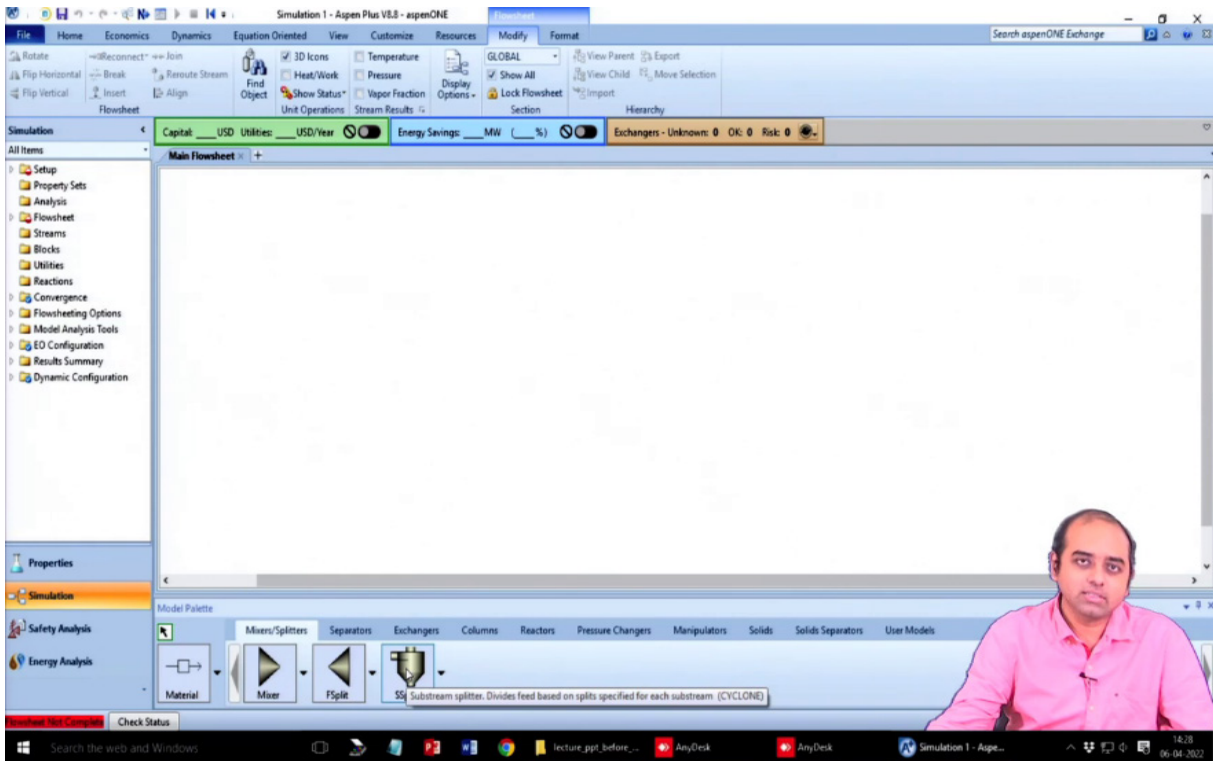
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For example, you can also work a little bit more on the units instead of, you can also set that the units here. Again, the specification, and now the next part are the main tab is the simulation tab.

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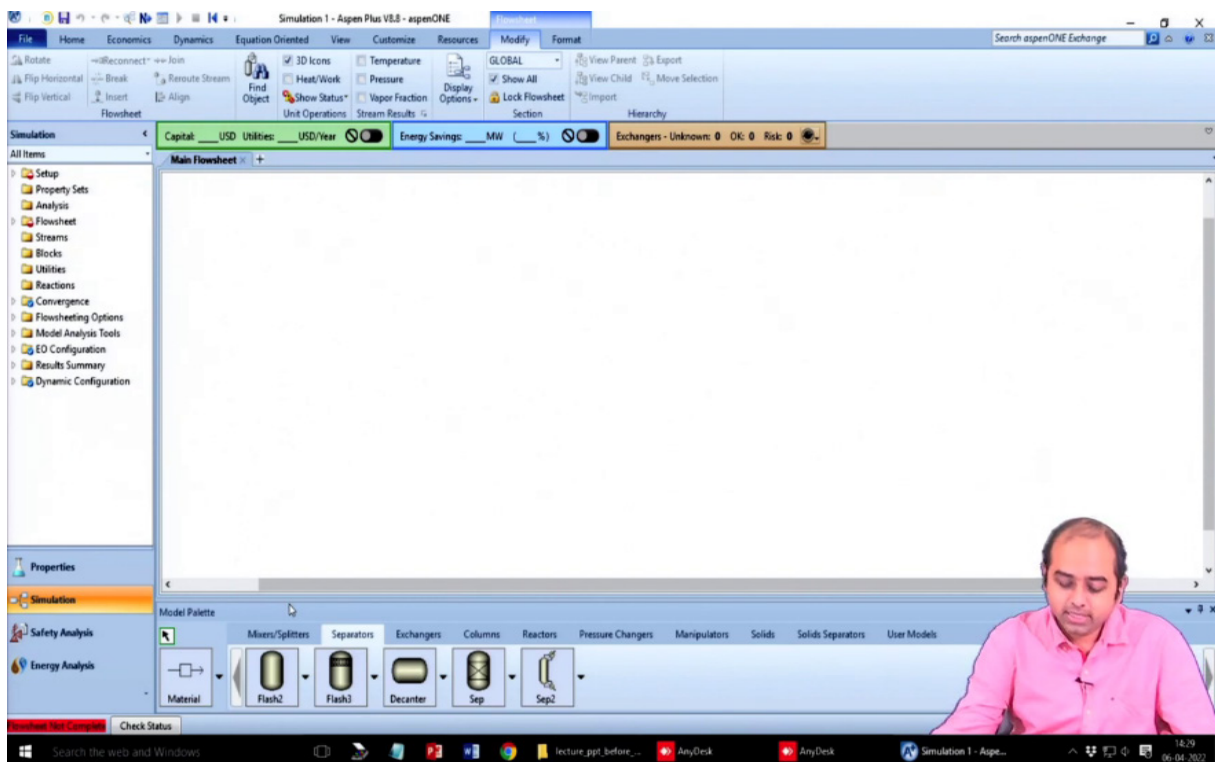


So, if you click the simulation tab on the left-hand side, you will see that there are different you know, items which are displayed on the left-hand side. And the window that is open is the flow sheet. Now at the bottom of this flow sheet, you will see that there are different types of unit operations. So, for example, these are called at the bottom. These are actually the

different elements of the different unique processes. I mean, their icons represent what type of unique processes they are.

So, the first one goes by the mixer. So, mixer is combination of merger is essentially combination of two or more streams into one. The next one is the splitter. So, again, splitter is of two types. One is the F Split, and one is the S Split. And if you move over the, over the mouse over that particular icon it will tell you that what is the, just a one line description of what does it, it means. So, splitter is essentially splitting one stream into two or more streams.

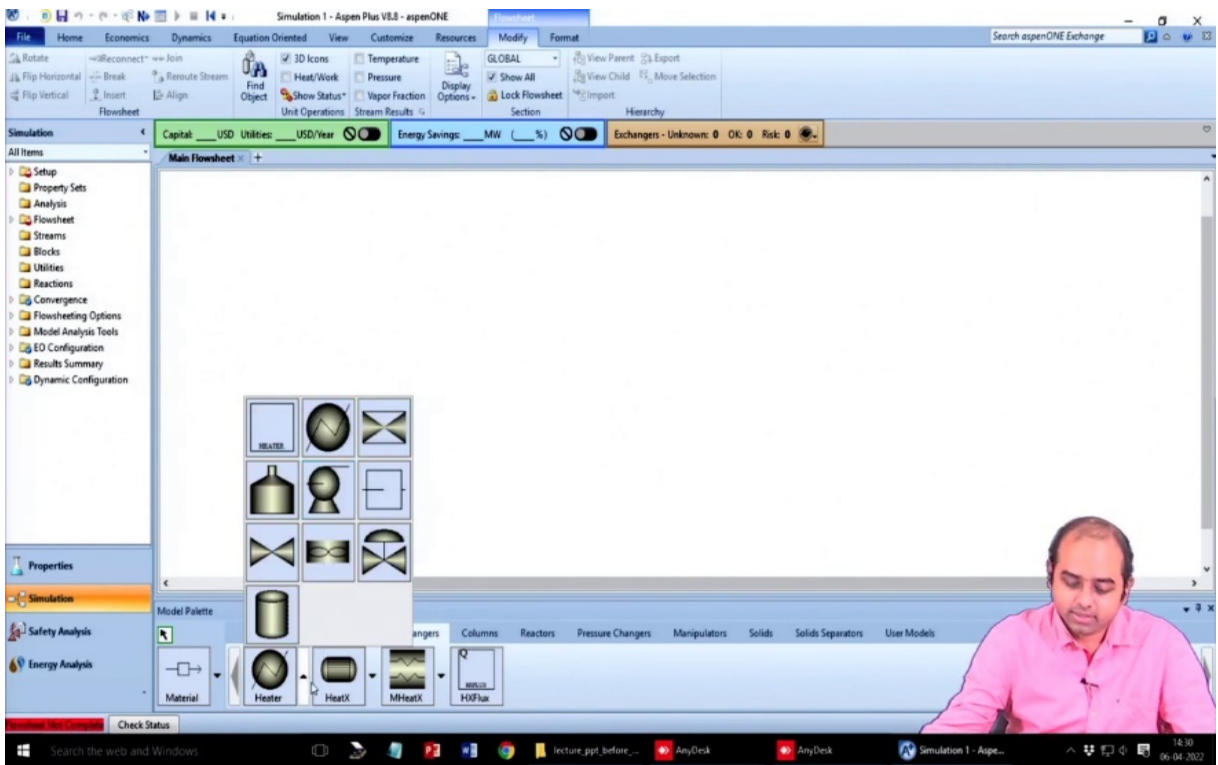
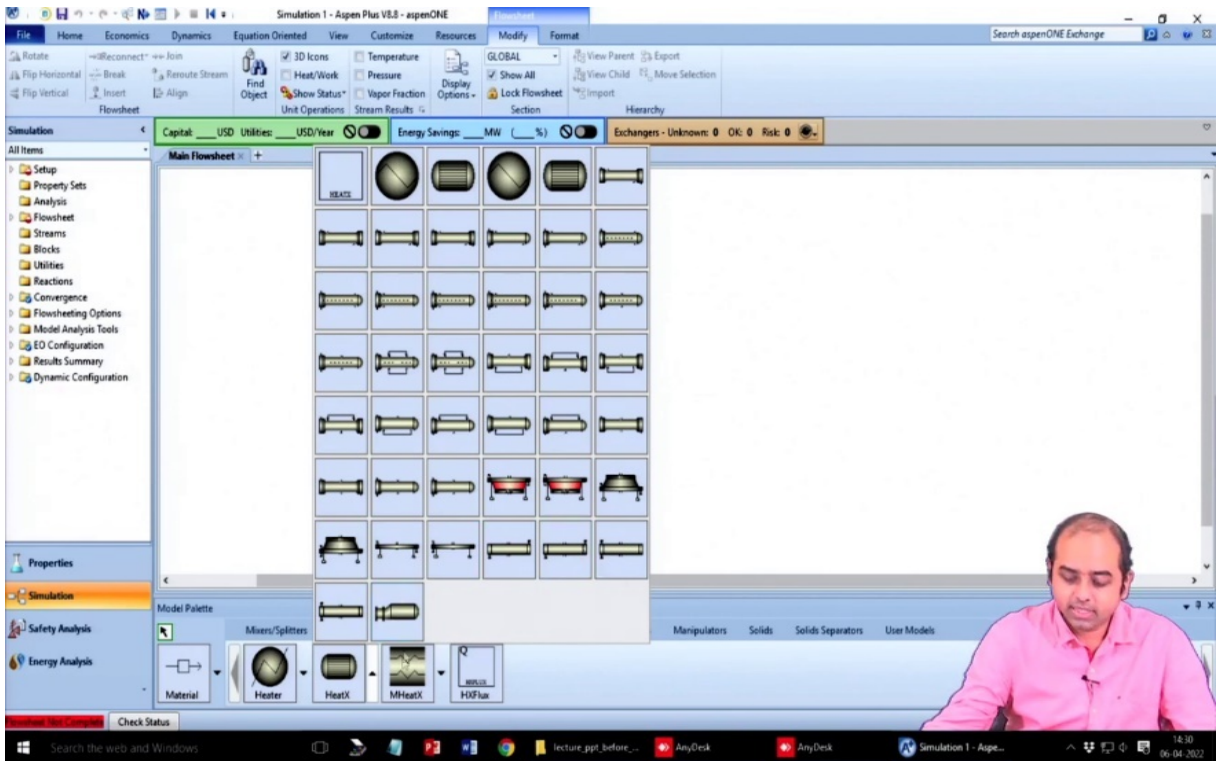
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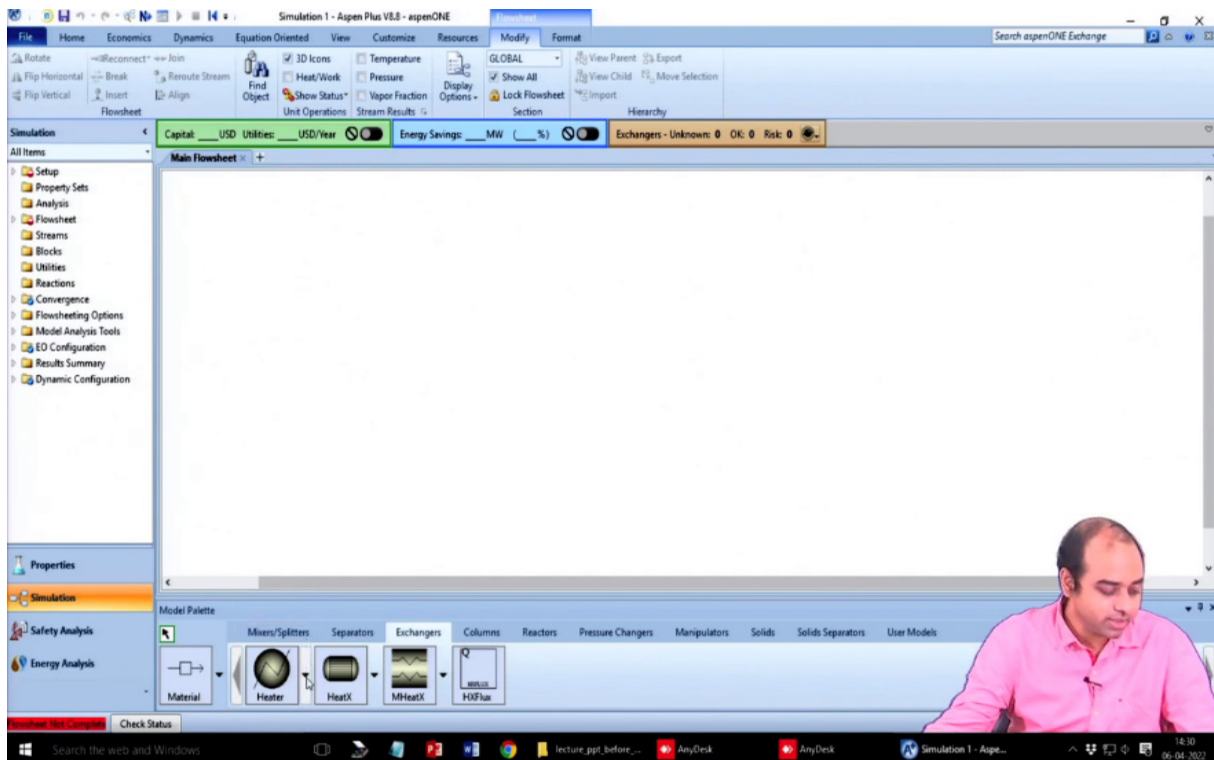


The next tab is a separator. And in the separator even see, there are different types of separators are present and please do not get confused with them as the distillation column. So, there is also another tab known as the distillation and column, which essentially presents the distillation column.

So, separator is essentially the flash. So, if you are selecting this Flash2, it essentially means, rigorous vapor, liquid, or two phase or vapor liquid split. And if you are selecting Flash3, it is essentially having three output streams. Next is the decanter is to separate two liquid stream. Sep is Sep and Sep2 are essentially separation based on flow and purities.

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Now, going to the heat exchangers. The first one is the heater. Please note that there is no cooler. So, heater can also be in the negative direction, with the negative value can also act as a cooler. And then next we have the heat exchanges. And if you also click the down arrow, you will also see there are several types of heat exchanges present, which can be used in this case.

So, this is I mean, these are the different types we will not go into too much of details. And there is something you can always look into from the, from essentially from the documentation. And heaters also have several types. Whether it is a block heater, whether it is this free energy heater, throttler, et cetera. All these types are there.

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Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources Modify Format

Simulation Capital: ___USD Utilities: ___USD/Year Energy Savings: ___MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet

Model Palette

Mixers/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Models

Material DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac ConSep BatchSep

Shortcut distillation design using the Winn-Underwood-Gilliland method (ICONT1)

Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources Modify Format

Simulation Capital: ___USD Utilities: ___USD/Year Energy Savings: ___MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

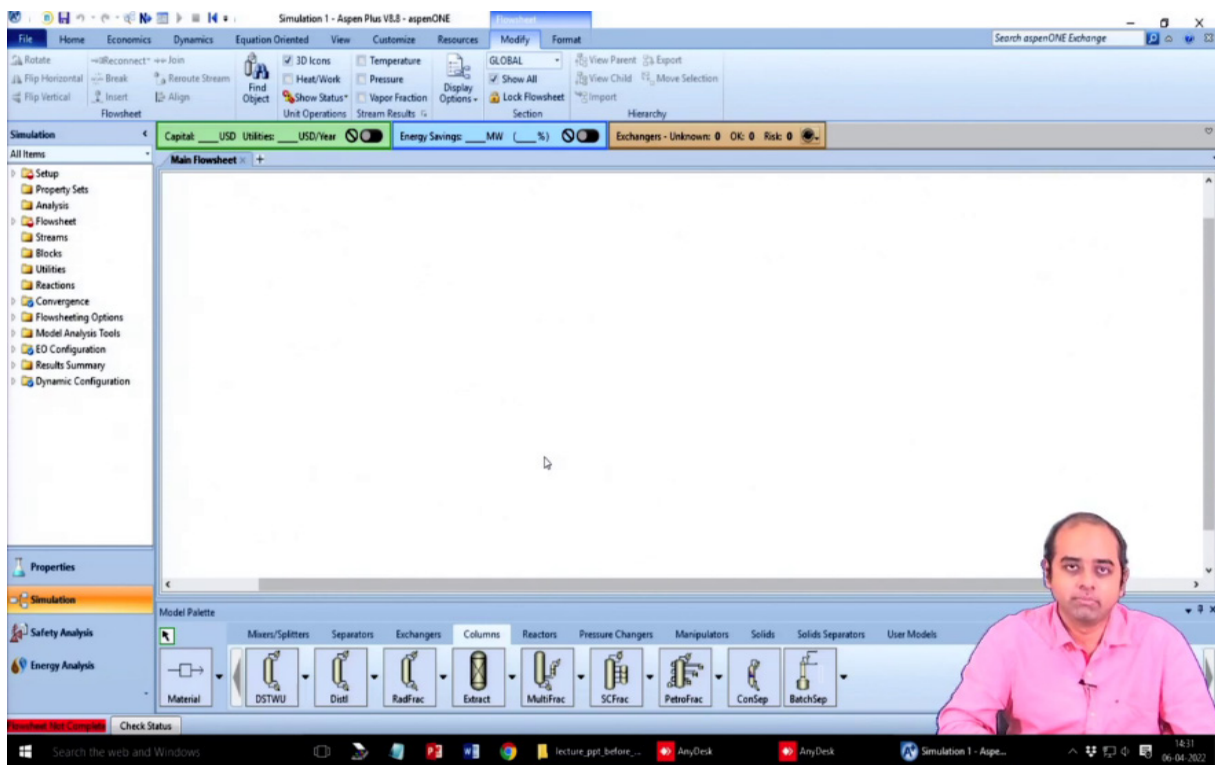
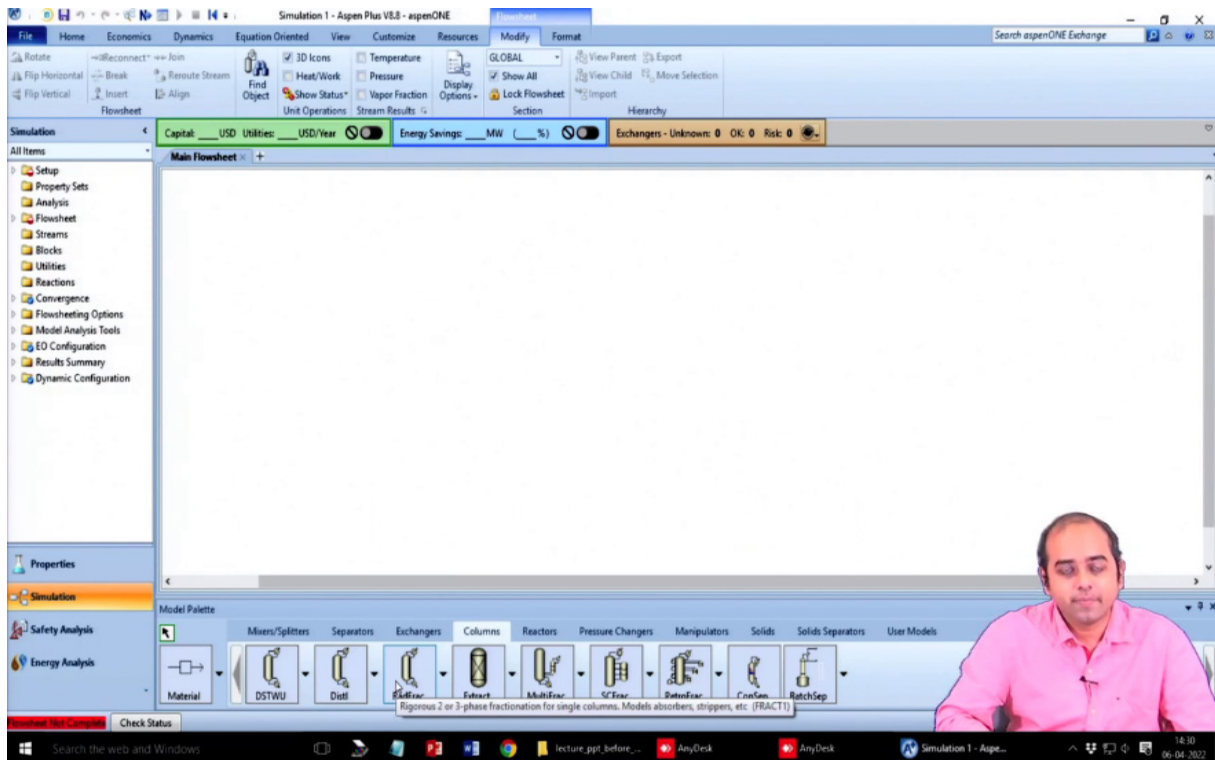
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Material DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac ConSep BatchSep

Shortcut distillation rating using the Edmister method (ICONT1)

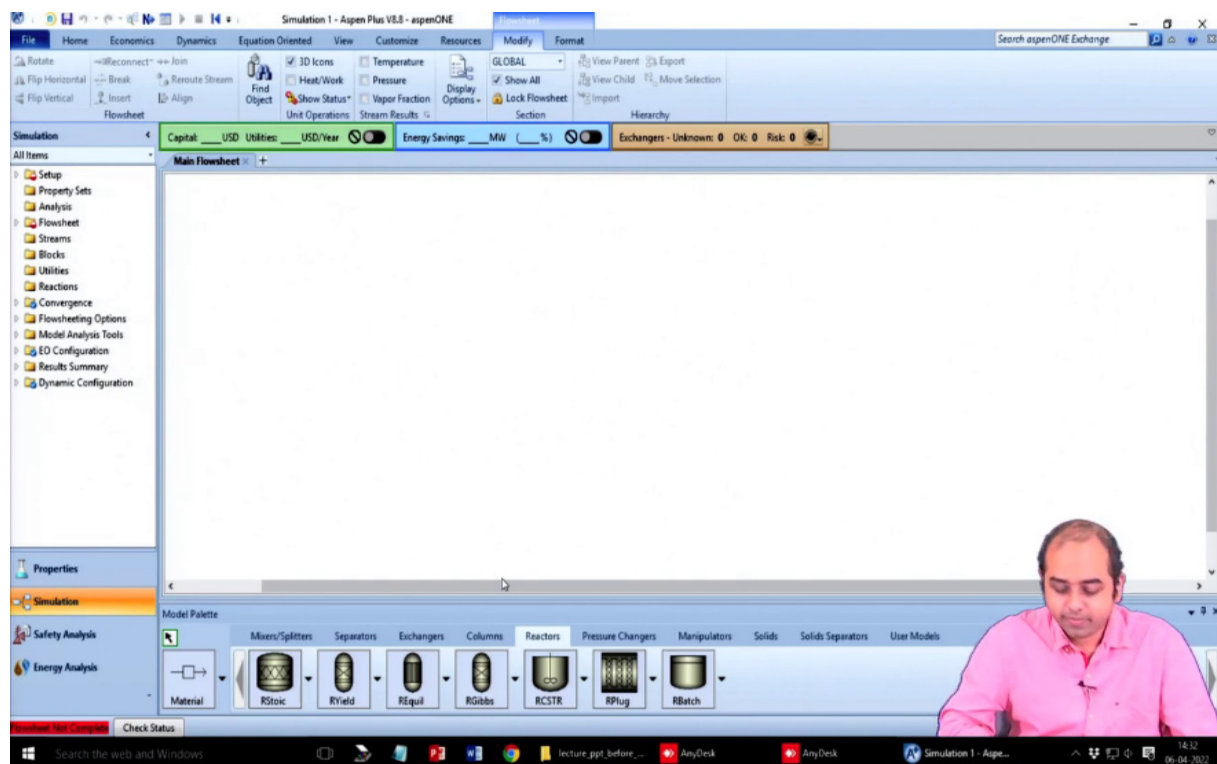


Next important part is the column. And in the column, we will see that there are different types of column. The first one is the DSTWU. So, the DSTWU is based on the shortcut method of the methods. So, calculation of the DSTWU is based on the Fenske-Underwood-Gilliland equations. Then the next one is essentially the, there is a one column called the

distillate and RadFrac is actually the most popular, distillation column where you can actually work a real life distillation column.

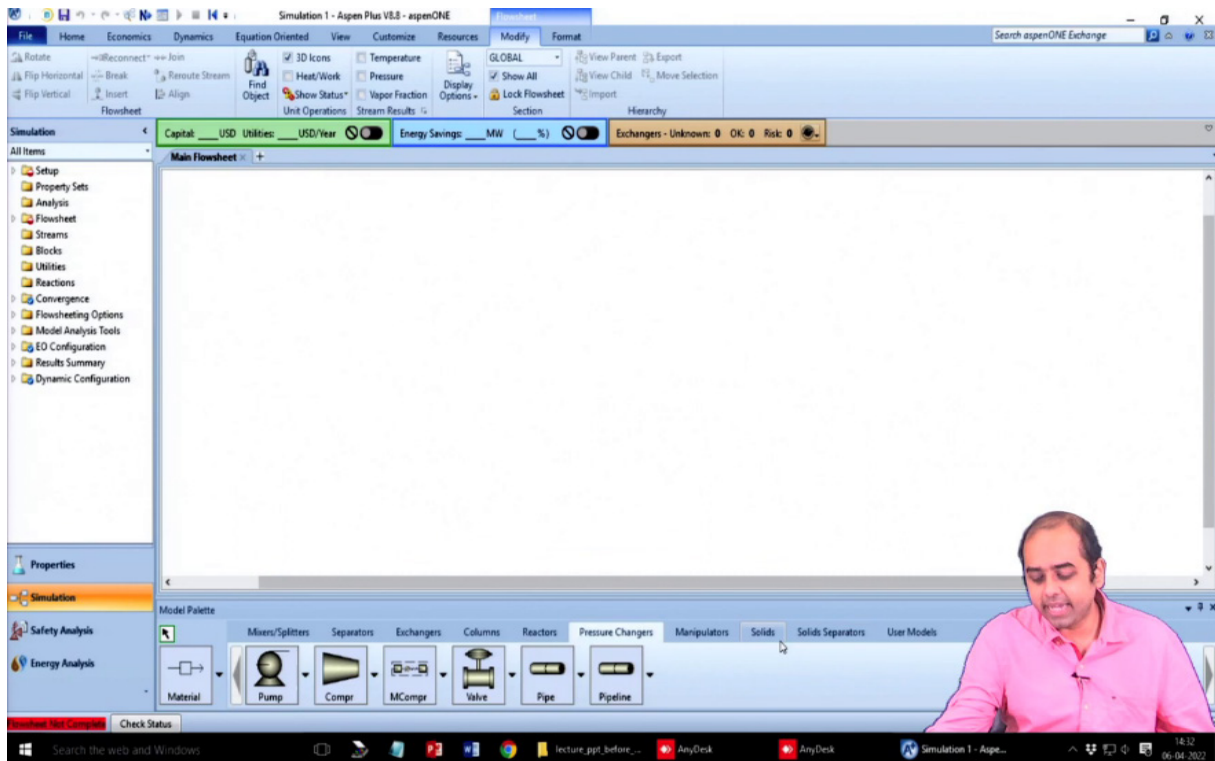
It uses the method of the bubble point method for the calculations. Then you have this multi fact method. It is this multi frac column, multi frac column is also very similar to RadFrac, but it has options for multiple exits or more number of fractionation outputs, which is more suitable for refining or petroleum industries. And multfrac generally operates with the under using the algorithm of the Newton Raphson of the simultaneous correction method. Then you have the other ones like Petrofac, and finally you have the batch separation of the batch distillation column.

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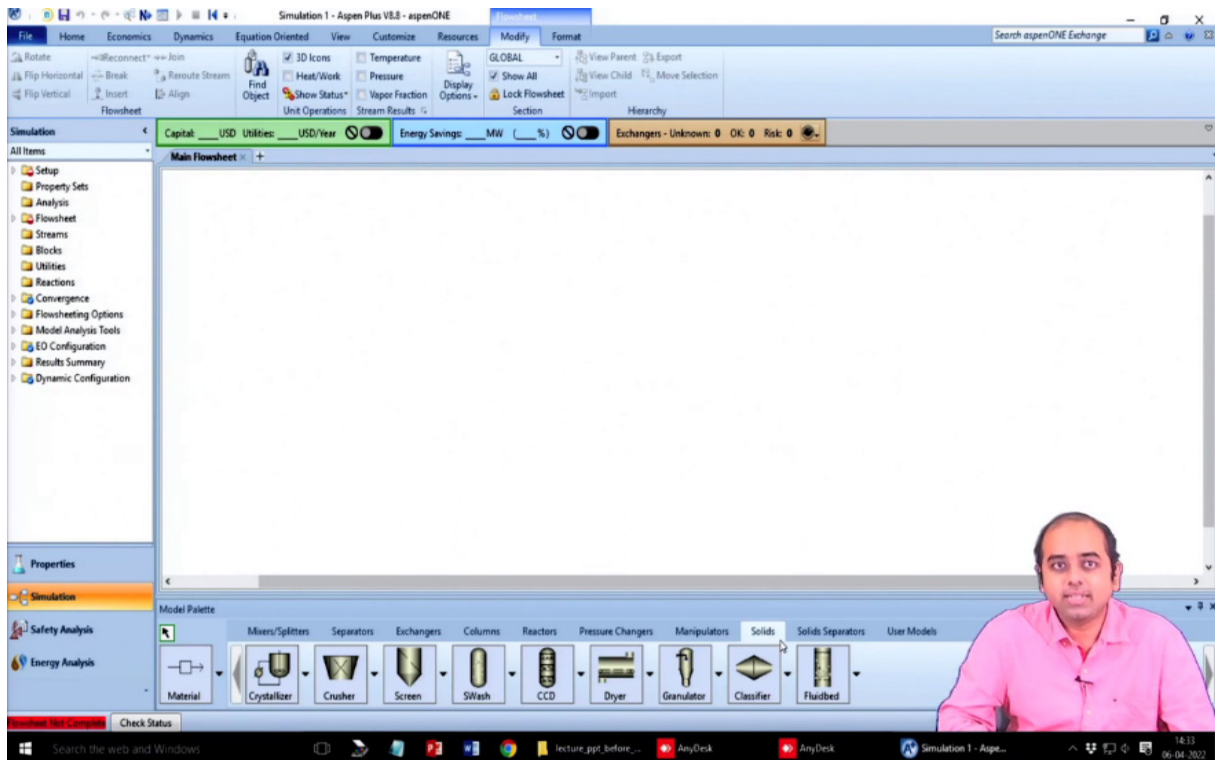
In the reactors also, you will see that there are several types of the reactors. The first one is the RStoic reactor, where you essentially specify a fractional conversion or the extent of the reaction. Next is, RYield. So, which is again, based on non-geometric reactions and based on the yield distribution, REquilibrium is based on the Gibbs free energy Is based on the equilibrium reactions. again, R Gibbs is also based on the free energy minimization of the reaction and with the determination of all possible reactions, including multi-phase reactions, then you have the CSTR type reactor, RPlug reactor, and the RBatch reactor mean it is, it is self explanatory by their names.

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Next tab is the Pressure Changes. So, by pressure changes, you can easily understand you have all the essentially these are the different sort of unit operations, which are very vital for changing the pressure of the streams. So, for pump, you have then compression multi-stage compression, then you have valve and different pipeline components, et cetera. If you want to calculate further in detail calculation of the pipe loss, pressure drop of the pipe, steam, friction, et cetera. Then there are some more, these tabs in this case.

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For example, the solid, so solid separators, like crystallizers, then we have cyclone separators then we have screen, fluidised bed, dryer, unit separation valves, solid particles. These modules are, these blocks are also peasant. Another question is that how to use these blocks? So, ideally you will select one of the blocks and you will place it in the mainstream. Sorry, the main flow sheet.

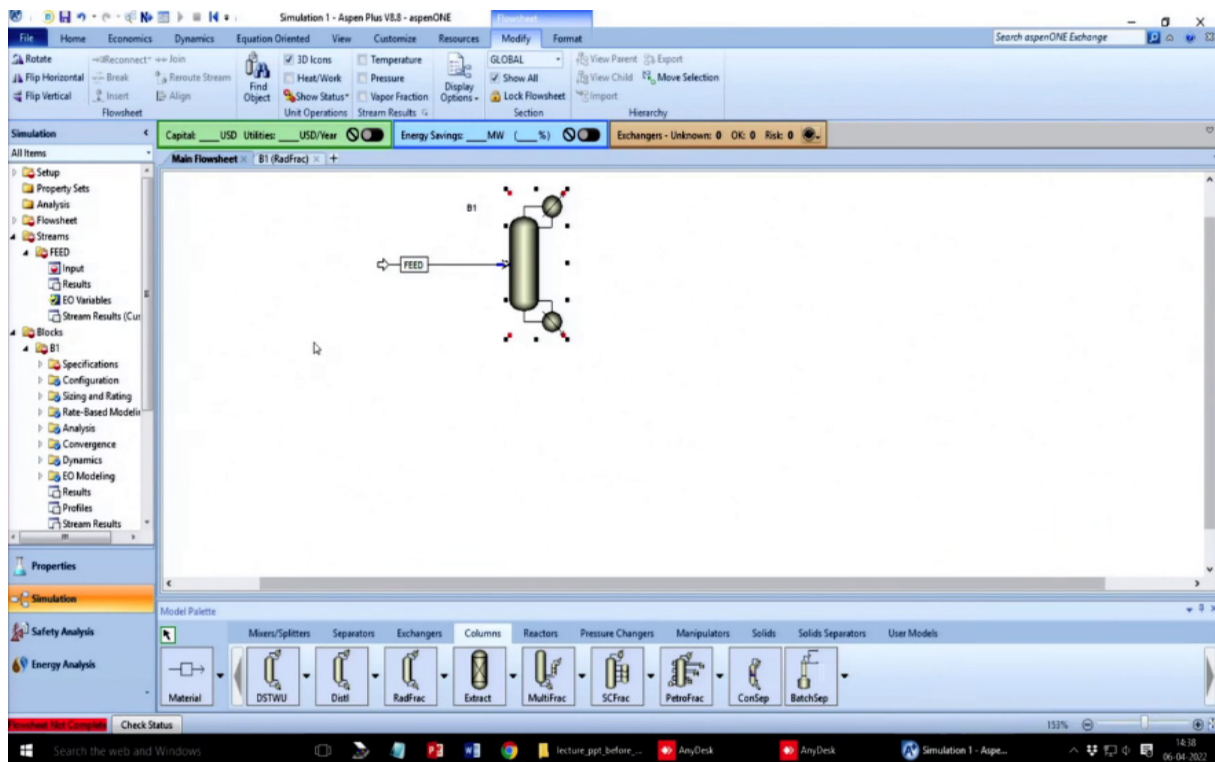
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The screenshot displays the Aspen Plus V8.8 - aspenONE software interface. The main window is titled "Simulation 1 - Aspen Plus V8.8 - aspenONE". The top menu bar includes File, Home, Economics, Dynamics, Equation Oriented, View, Customize, and Resources. The simulation status bar shows "Capital: ___USD", "Utilities: ___USD/Year", "Energy Savings: ___MW (%)", and "Exchangers - Unknown: 0 OK: 0 Risk: 0". The left sidebar contains a tree view with categories like Setup, Analysis, Flowsheet, Streams, and Blocks. The main workspace is titled "Main Flowsheet > FEED (MATERIAL) >". The "Specifications" panel is active, showing "Flash Type" set to "Temperature" and "Pressure". The "State variables" section includes fields for Temperature (C), Pressure (bar), Vapor fraction, Total flow basis (Mole), Total flow rate (kmol/hr), and Solvent. The "Reference Temperature" section includes "Volume flow reference temperature" and "Component concentration reference temperature", both set to "C". A "Composition" table is visible with columns for "Component" and "Value", and a "Total" field set to 0. The "Model Palette" at the bottom shows various unit operation icons such as Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, and User Models. A video feed of a man in a pink shirt is overlaid in the bottom right corner of the software window.

The screenshot displays the Aspen Plus V8.8 - aspenONE software interface. The main window is titled "Simulation 1 - Aspen Plus V8.8 - aspenONE". The top menu bar is the same as in the previous screenshot. The simulation status bar shows "Capital: ___USD", "Utilities: ___USD/Year", "Energy Savings: ___MW (%)", and "Exchangers - Unknown: 0 OK: 0 Risk: 0". The left sidebar is the same. The main workspace is titled "Main Flowsheet > B1 (RadFrac) >". The "Configuration" panel is active, showing "Setup options" with "Calculation type" set to "Equilibrium", "Number of stages" set to 1, "Condenser" set to "Kettle", "Reboiler" set to "Kettle", "Valid phases" set to "Vapor-Liquid", and "Convergence" set to "Standalone". The "Operating specifications" section includes "Distillate rate" (Mole, kmol/hr), "Reflux ratio" (Mole), and "Free water reflux ratio" (0). The "Model Palette" at the bottom is the same as in the previous screenshot. A video feed of the same man in a pink shirt is overlaid in the bottom right corner of the software window.

The screenshot displays the AspenONE software interface for a simulation. The title bar reads "Simulation 1 - Aspen Plus V8.8 - aspenONE". The menu bar includes File, Home, Economics, View, Customize, Resources, Modify, and Format. The simulation status bar shows "Capital: ___ USD", "Utilities: ___ USD/Year", "Energy Savings: ___ MW (%)", and "Exchangers - Unknown: 0 OK: 0 Risk: 0". The left-hand navigation tree shows a hierarchy of items including Setup, Property Sets, Analysis, Flowsheet, Streams, FEED, Input, Results, EO Variables, Stream Results, Blocks, B1, Specifications, Configuration, Sizing and Rating, Rate-Based Model, Analysis, Convergence, Dynamics, EO Modeling, Results, Profiles, and Stream Results. The central area shows a process flow diagram with a "FEED" stream entering a "RadFrac" column labeled "B1". The model palette at the bottom includes categories like Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, and User Models. A person in a pink shirt is visible in the bottom right corner of the screen.

This screenshot shows the same AspenONE software interface as the first image, but with the "Run (F5)" button highlighted in the menu bar. The simulation status bar and navigation tree are identical. The central process flow diagram remains the same. The person in the pink shirt is now resting their chin on their hand, appearing to be in a thinking or listening posture.



For example, I choose this RadFrac, I just do a left click. And then if I click it here, a RadFrac will be selected. And then I have to select, if I click the material button, it will ask me to specify the different mandatory streams for this distillation column. And as you can understand, I must specify the minimum requirement is to have 1 feed stream, 1 bottom outlet, 1 top outlet, and 1 is sort of the reflex over there. The blue ones are essentially the optional ones.

So, this is what you see that these are the common stream connections that needs to be made. So, for example, if I want to add a stream, so I have to click left click, and then I have to drag and get it to the connect it to the inlet of the distillation column. So, if I do this, then it will automatically show that this connection has been made, but still it is not showing it properly.

So, now if you see one arrow is there and it shows that the stream is numbered as stream 1. And this minimum requirement of the inlet stream is satisfied, but still the other streams are remaining. If you see it here that there is still, there are some red, so other streams needs to be connected. So, these are all about the stream connections and you can always reconnect a stream, delete a stream, add a new connection.

All these things can be done. Just be careful on how you click your mouse and how you connect them. But please make sure that once the connection is done properly the software will not show the red coloured stream options because that the mandatory requirements are

fulfilled. So, often people do a mistake that you do not connect it properly to the desired location. And even though you feel that visually it appears that a stream is drawn, but it is not actually connected. So, there is a disconnected stream.

So, that is something you need to be careful about. You can always rename your stream. So, let us say this stream is something which I can rename as like 'feed'. So, up to 8 characters are allowed for the stream naming and if I double click on this stream, it will ask for the specifications. Now, of course we have not specified the chemicals, et cetera. So, these things are not coming in the picture again, similar, if I double click on the distillation column, it will ask for the specifications and unless the required specifications are provided, it will be marked as red.

So, this is the overview of the general layout of the software. So, after all the streams, all the blocks or all the unique operations are actually specified in your main flow sheet, the next step is to run the simulation. So, then the calculation can be done. So, how do you run the simulation? So, if you go to the top, there is one small icon. so here the run option is not activated because the required inputs are not complete.

So, once all the required inputs are complete automatically, we will see at the top, there is a run option. So, I think this is the run option or a F5 you can press. And before pressing the this run button, you need to initialize your system or the initial values for, so this is related calculation. So, iterative calculation works by continuous iteration based on the initial guess. So, some initial guess has to be provided. And in general, the software takes that by itself, depending on the kind of values that we have provided in the inputs.

So, at the bottom, this status message that you see that the flow sheet not complete because the required specifications are not done again, required stream connections are not made. And after the required connections are done, it will show that initialization is not done. So, then you have to click for the system initialization where this icon will be there at the bottom. And then it will say that the required installation is done.

And then after you click, it will say that the run is complete and results are available. So, this is how it works. So first, you have to prepare your flow sheet, make all the stream connections specify all the required input information for the streams, as well as for the different units, then initialize your problem and then run your problem and check for the results. So, this is how the sequence of the operation works. Now, let us look into the problem that we are trying to solve for today.

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Factors which affect distillation

- Number of trays
- Reboiler duty
- Reflux ratio
- Boilup flow rate
- Feed flow rates
- Feed location

Goals

- Product purity
- Energy efficiency

The diagram illustrates a distillation column with a reboiler and condenser. The column is divided into an Enriching Section (top) and a Stripping Section (bottom). Feed enters between the two sections. The top product is Distillate, which goes through a Reflux Drum and is returned to the column as Reflux. The bottom product is Bottoms. A Reboiler at the base provides Heat In and Heat Out. A Condenser at the top provides Heat In and Heat Out.

So, in general, a distillation, this is a problem about distillation column. We all know that the factors which affect the distillation processes are the reboiler duty reflux ratio, number of stages, feed, stage location, feed flow rates then the condenser load, these are generally the factors which affect presence of an internal third, component like that. And generally, the things that we target for is what is the product purity either in the top or at the bottom, and what is the energy efficiency of the system.

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Problem 1: Purification of methylcyclohexane by distillation

Methylcyclohexane (MCH) and toluene form a close boiling mixture that is difficult to separate by simple binary distillation. Phenol is generally used as an entrainer in this case. The purity of the recovered MCH depends on the phenol input flow rate.

Phenol 1200 lbmol/hr
220°F
20 psia

MCH 200 lbmol/hr
220°F
20 psia

Toluene 200 lbmol/hr
220°F
20 psia

No. of equilibrium stages 22
Total condenser
Reflux ratio 8
Distillate rate 200 lbmol/hr
Condenser pressure 16 psia
Reboiler pressure 20.2 psia

So, let us look into this problem on purification of this methylcyclohexane and toluene mixture by distillation. So, generally MCH this methylcyclohexane and toluene form, a constant close boiling mixture. So, beyond a certain mole fraction of toluene sorry, methylcyclohexane, it is not possible to separate them by distillation because they form a constant boiling mixture azeotrope.

So, and then, so that is around 0.75 of the MCH. So, beyond 0.75 mole fraction of metal is not possible to separate it from, to, because it forms almost close boiling mixture. And to circumvent this problem what you do is that you use phenol as an entrainer, so phenol is a third component that is inserted or introduced into the system so that this the thermodynamics or this phase separation can be done to a greater extent.

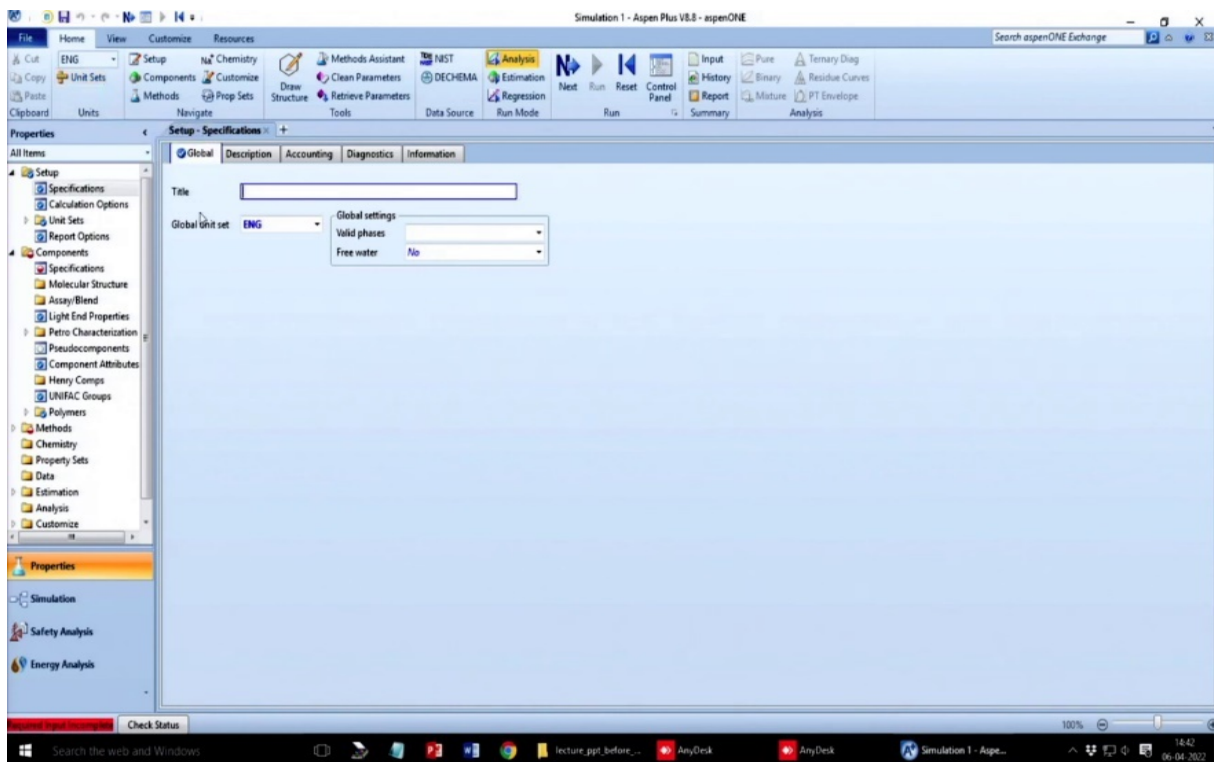
And of course, it goes without saying that the purity of the, methylcyclohexane depends on the phenol or the proportion of phenol in the overall system. So, phenol does not take part in the process, but essentially phenol helps in changing or altering the phase composition or the phase diagram, in fact. So, let us look into this problem so first how will we do? So, first we will try to look into the, X Y diagram of the methylcyclohexane and toluene then using these two only let us try to do distillation.

And it, us try to see that what is the optimum number of stage, what would be the appropriate feed location, et cetera, although the feed location is already specified. So, we can see an optimization of the changing this number of stages, et cetera, as a general case. And then finally we introduce the phenol and try to vary flowrate and see that under what flow rate, the maximum cyclohexane can be recover.

So, all the rest of the specifications are already mentioned in this problem that you can consider total number of stages to be 22, reflux ratio 8. But these are the parameters that you can do a variation, parametric variation, and can check that which is the most optimal value. So, this is the first problem we are going to study.

So, let us look into that, let us try to insert our distillation column, connect the appropriate streams and try to find out what is the composition for some selected conditions. And then we slowly build on that problem with the introduction of phenol and trying to do this sensitivity variation by altering the flow rates or the number of stages, et cetera.

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Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home View Customize Resources

Properties Components - Specifications

Find Compounds

Search Criteria

Name or Alias:

Compound class:

Molecular weight: From To

Boiling point: From To

Compounds found matching the specified criteria

Compound name	Alias	Databank	Alternate name	MW	BP <F>	CAS number	Compound class
METHYLCYCLOHEXANE	CTH14-6	APV88.PUR	Methylcyclohexane	98.18	213.6812	108-87-2	ALKYLCYCLOHEX
1,1-DIMETHYLCYCLOHEXANE	CSH16-1	APV88.PUR	1,1-Dimethylcyclohexane	112.2	247.1900	590-66-9	ALKYLCYCLOHEX
CIS-1,2-DIMETHYLCYCLOHEXANE	CSH16-2	APV88.PUR	1,2-Dimethylcyclohexane	112.2	265.6220	2207-01-4	ALKYLCYCLOHEX
TRANS-1,2-DIMETHYLCYCLOHEXANE	CSH16-3	APV88.PUR	1,2-Dimethylcyclohexane	112.2	254.1740	6876-23-9	ALKYLCYCLOHEX
CIS-1,3-DIMETHYLCYCLOHEXANE	CSH16-4	APV88.PUR	1,3-Dimethylcyclohexane	112.2	248.1620	638-04-0	ALKYLCYCLOHEX
TRANS-1,3-DIMETHYLCYCLOHEXANE	CSH16-5	APV88.PUR	1,3-Dimethylcyclohexane	112.2	256.0280	2207-03-6	ALKYLCYCLOHEX

Add selected compounds

Matches found: 14 (5 seconds)

Close

Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home View Customize Resources

Properties Methods

Method filter: COMMON

Base method: UNIFAC

Method name: UNIFAC

Modify

Vapor EOS: ESRK

Data set: 1

Liquid gamma: GMUFAC

Data set: 1

Liquid molar enthalpy: HLMX103

Liquid molar volume: VLMX01

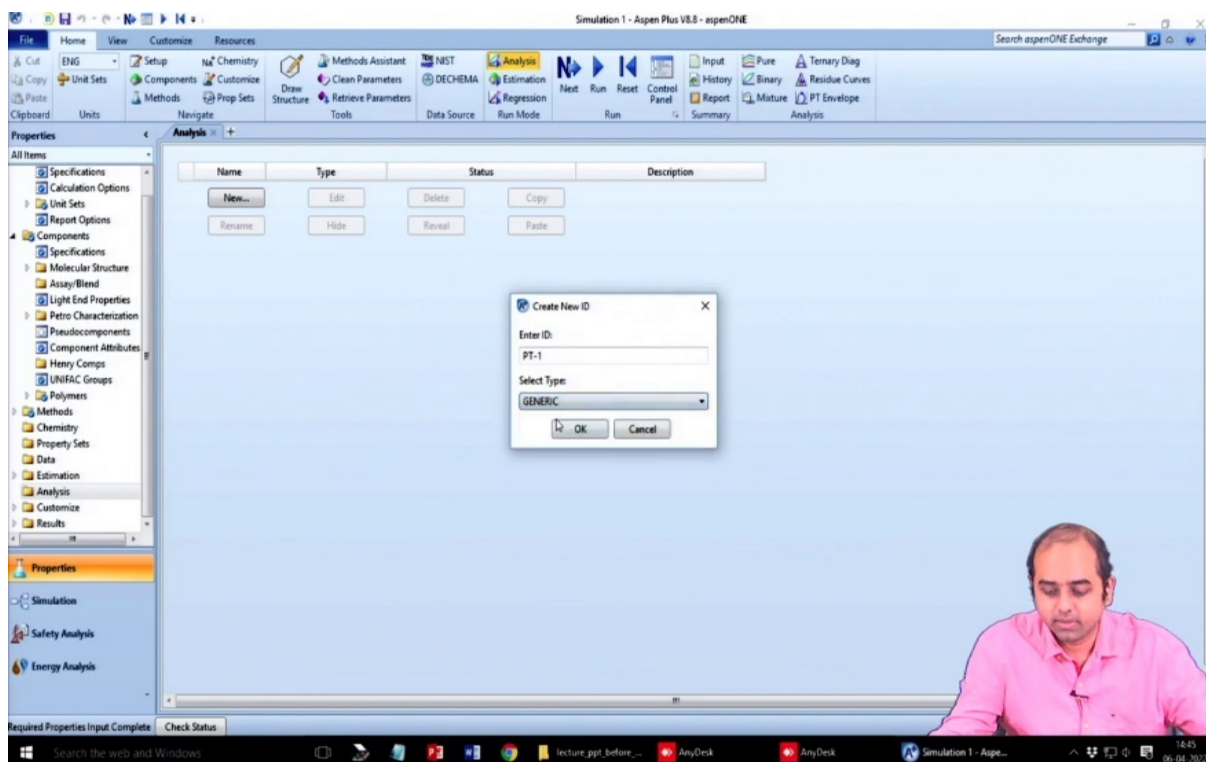
Heat of mixing

Poynting correction

Use liquid reference state enthalpy

Required Properties Input Complete

Check Status



So, first we will go to the properties. Let us select the unit as ENG, English units, because everything is specified in SI and, Fahrenheits and all. So, the specification, how do we find? So, we have to just type the name, the easiest way to find them, instead of going into the detailed wizard is to write the name, toluene, and then press enter. So, if that matches already, then it will show or automatically the software will fill up the rest of the information.

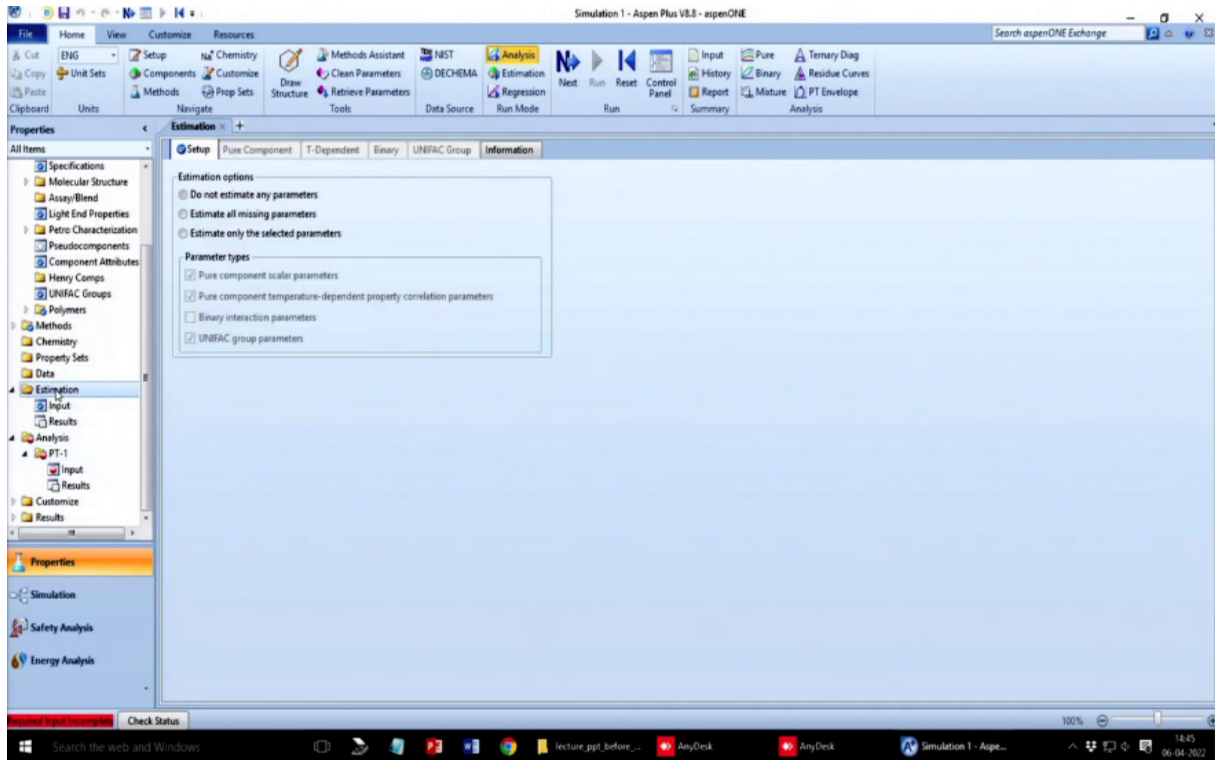
Like toluene is the name given by us, but the chemical name is already written now is also toluene. So, that is the easiest way to find. If you write down the name of the chemical, it will easily find it, it will write all its formula and all other properties will also be automatically selected by the software or specified by the software. Next one is that methylcyclohexane. That is not coming. So, let us use that is a big one.

So, let us use the find wizard. Let us write any methylcyclohexane, and click on this find now. So, it will list on all the possible matches from its data bank. And you will see that the first one is what we are looking for actually, methylcyclohexane. There are others also, but that is the one which is the most likely match. Then also we have phenol. So, these three are the components which we will be working with.

So, once these are specified, the next thing to do is to work on the methods. In the base method, let us choose UNIFAC and all the specifications are done. So, when all the specifications are done, you see that on the left-hand bar or the left-hand block. There are no

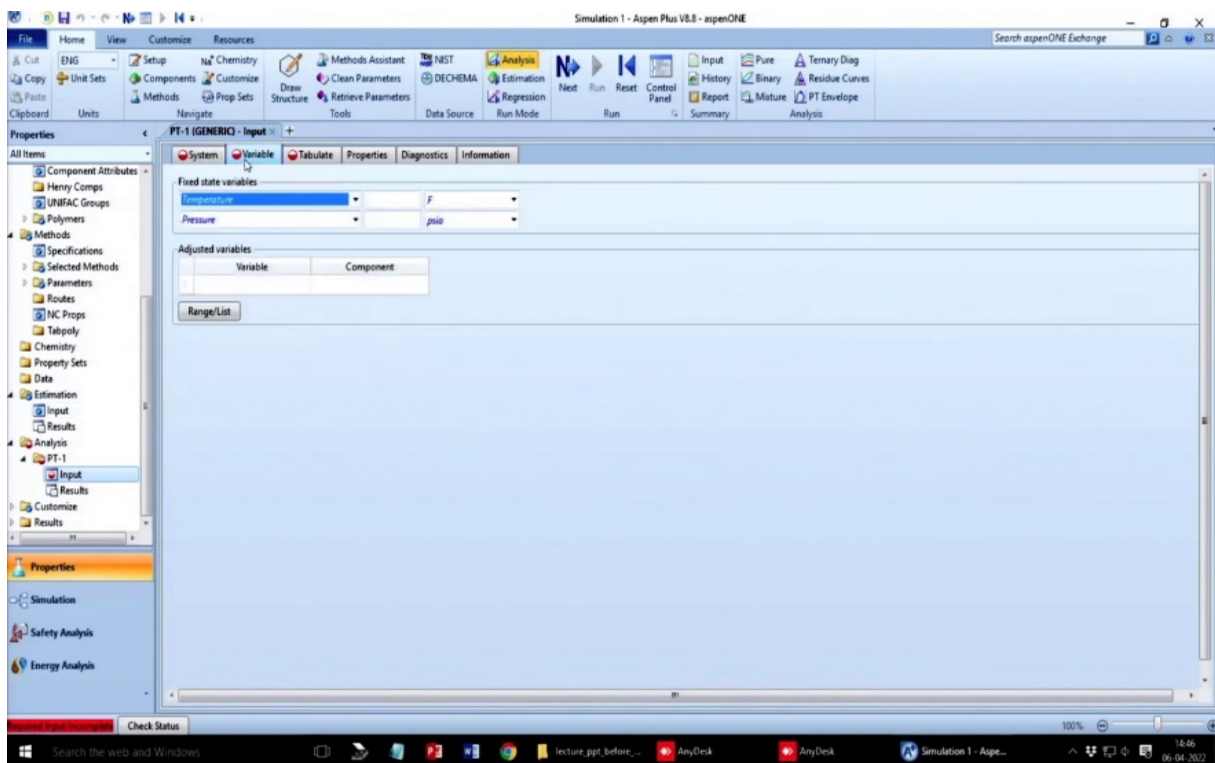
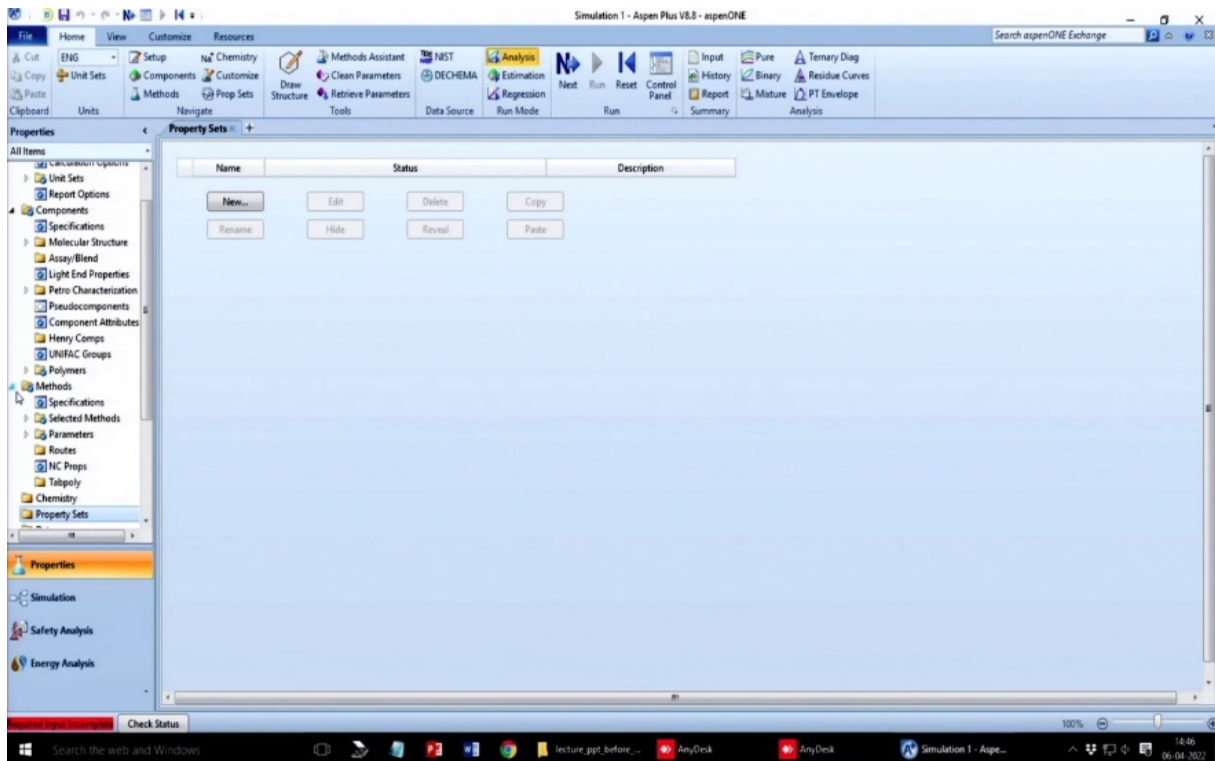
red buttons or red icons. Now, we can also do a quick check on trying to find out that T X Y diagram.

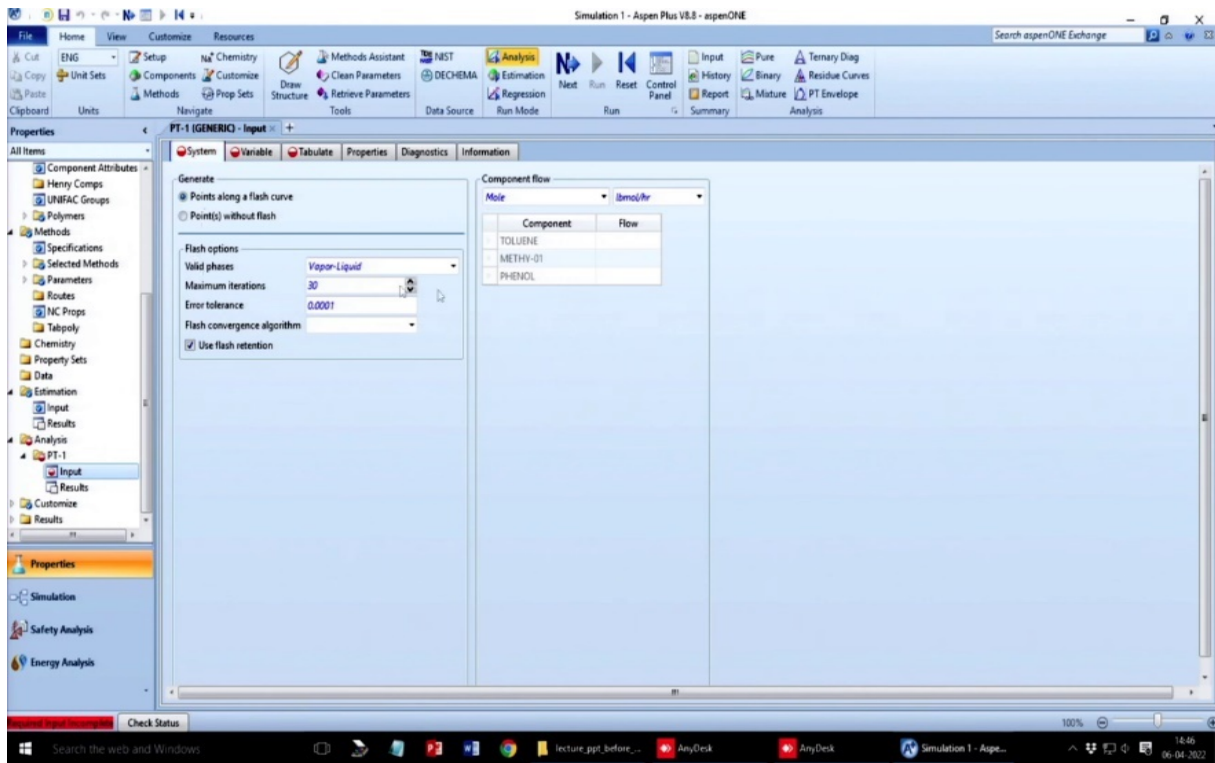
(Refer Slide Time: 24:04)



So, analysis will go, it is all in the property block now. We have not gone to the simulation part.

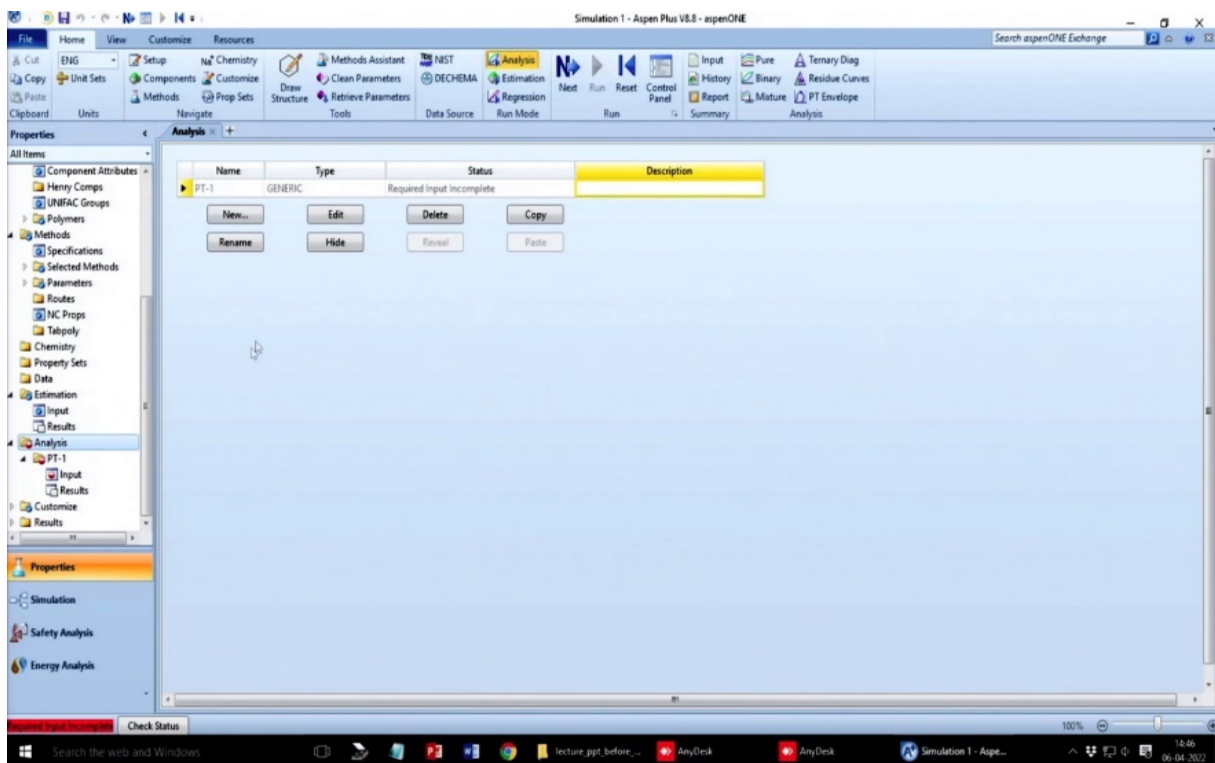
(Refer Slide Time: 24:19)

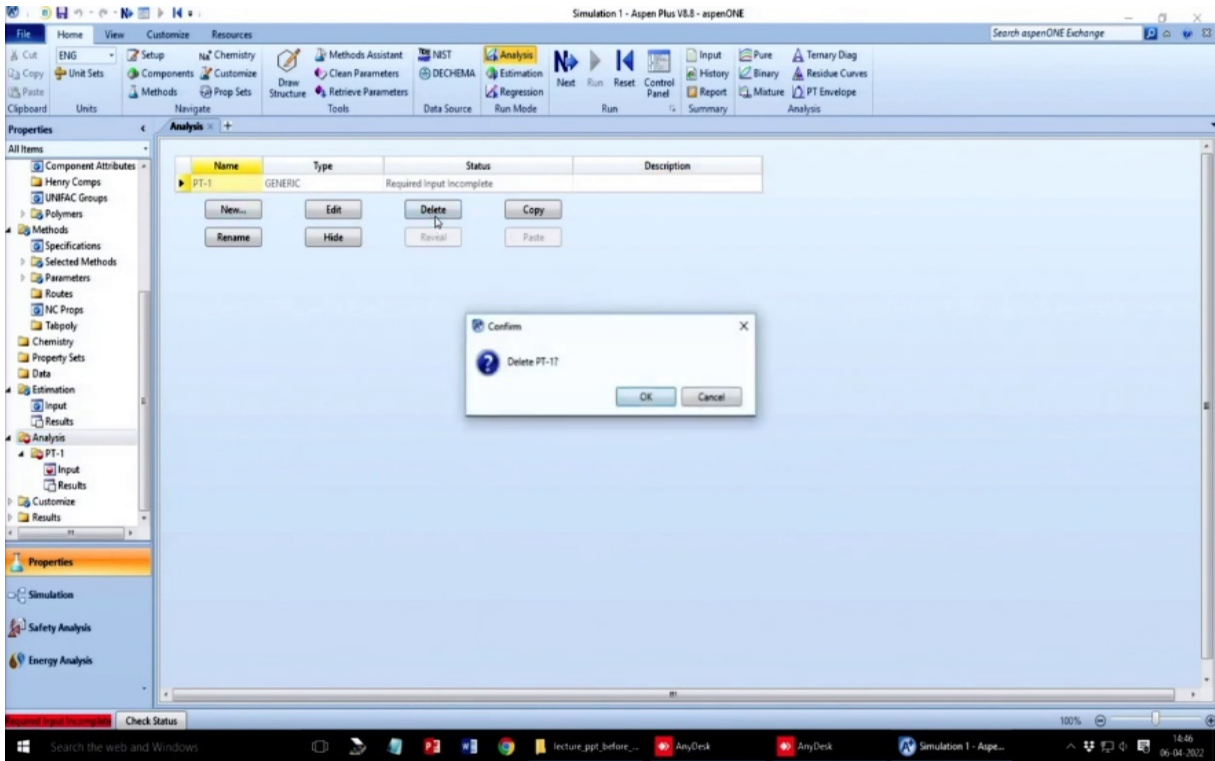




I do not think this is the one. No.

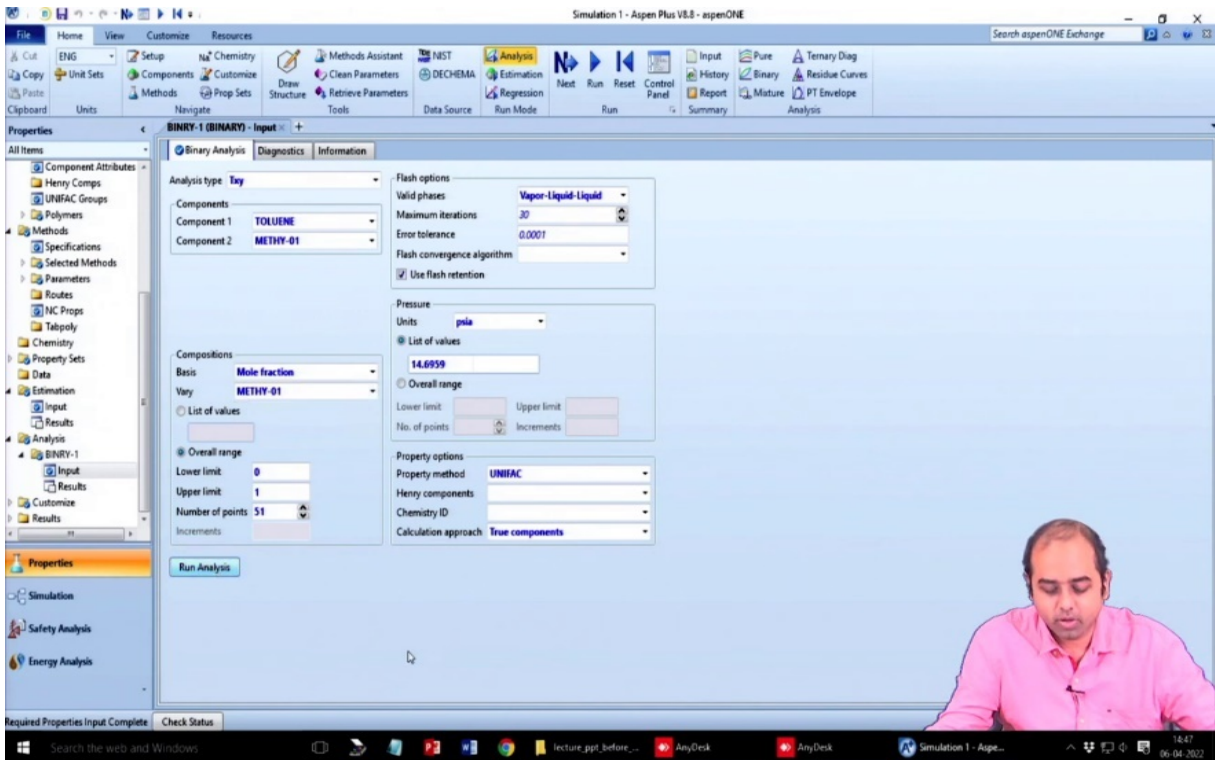
(Refer Slide Time: 25:08)





So, if you click on this analysis, let us delete that. And at the top, you will see that there is something known as the binary analysis, that icon is there.

(Refer Slide Time: 25:21)



So, if you click on that binary analysis, very easily, you will get the binary analysis block. It will show you the type of analysis as T X Y it can also to P X Y. Let say, I select, this

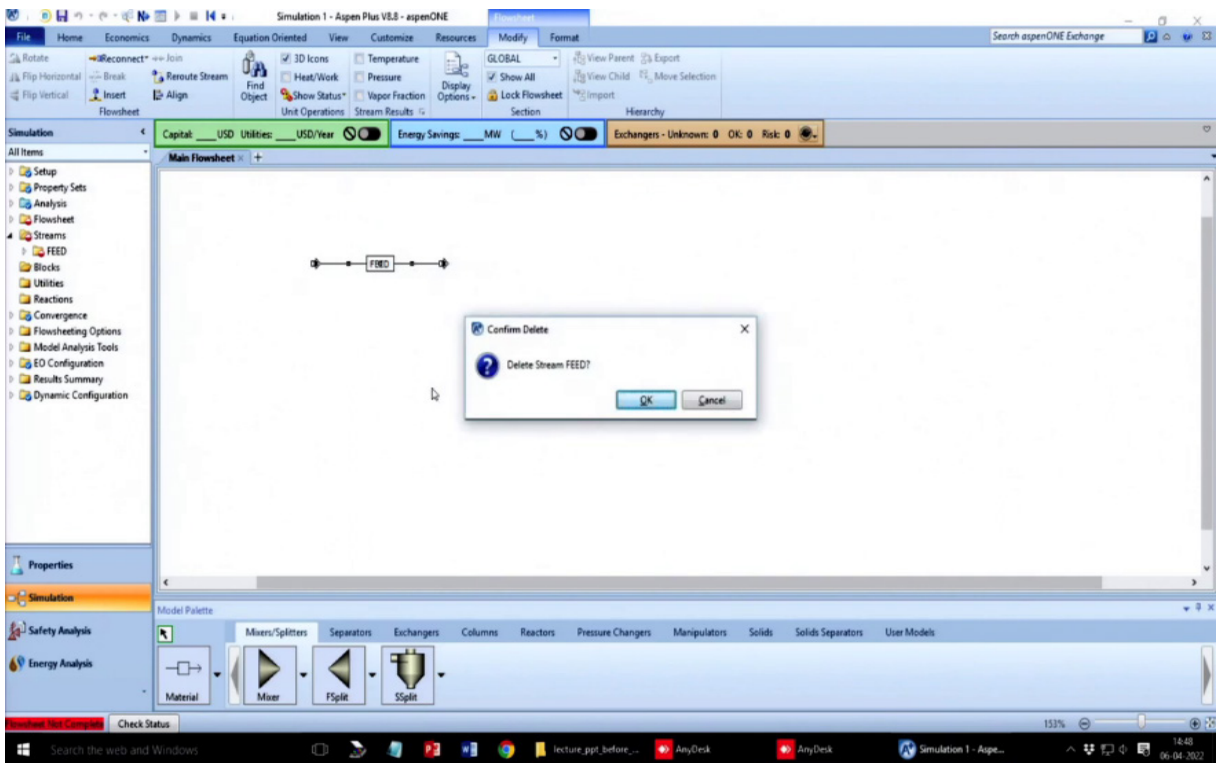
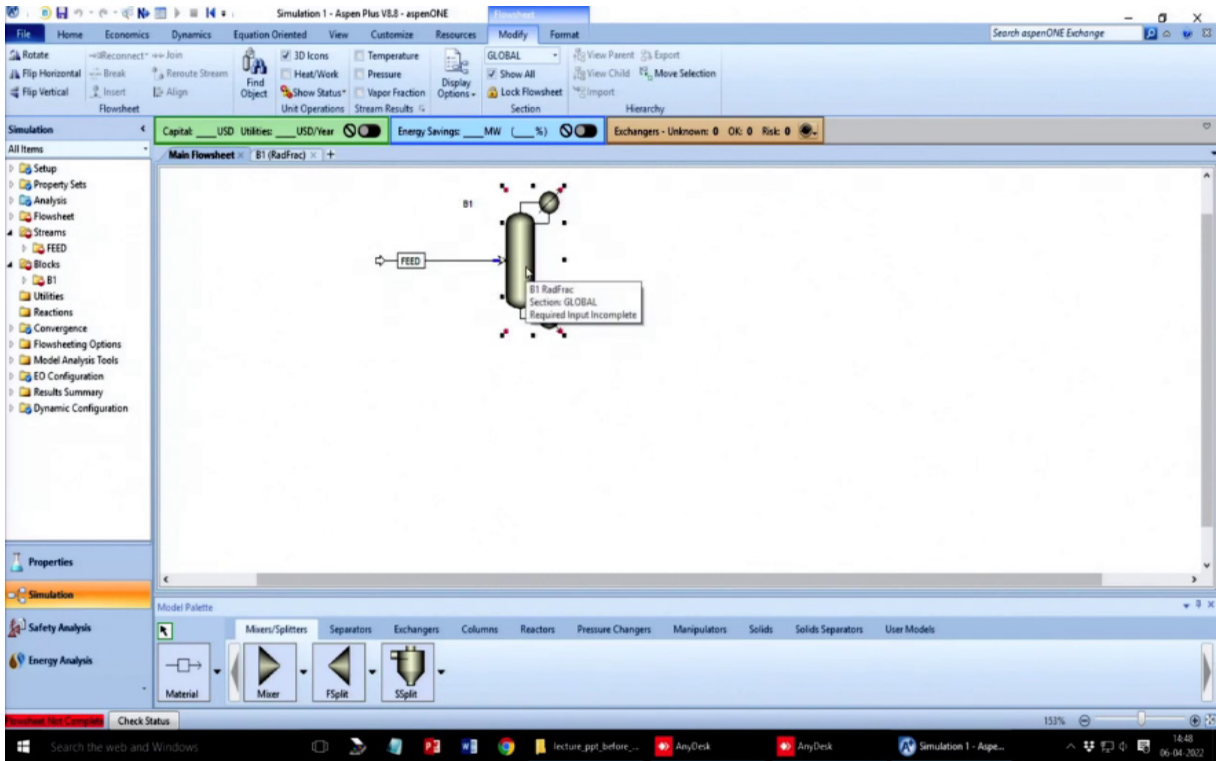
methylcyclohexane, which is marked as 0 1. And let say I vary the methylcyclohexane fraction. And now if I try to run analysis, it will show us a plot of the T X Y diagram.

(Refer Slide Time: 25:51)



So, this is the T X Y diagram. And if you look carefully here that beyond 0.75 the difference in the Y and the X phase composition of cyclohexane is very small. So, this is the part which shows that it is very difficult to separate or improve the vapor phase composition or enrich the vapor phase composition of the cyclohexane in methylcyclohexane mixture. Below that it is, it is the difference is quite strong. You can see it here itself. So, this is something I wanted to show that it forms a sort of azeotrope beyond 0.75, and after 8.8, it is almost same. So, from 0.75, it is not energetically feasible to separate them by distillation.

(Refer Slide Time: 26:57)



Simulation 1 - Aspen Plus V8.8 - aspenONE

Capital: ___ USD Utilities: ___ USD/Year Energy Savings: ___ MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet: FEED (MATERIAL)

Specifications

Flash Type: Temperature Pressure

State variables

Temperature: 220 F
 Pressure: 20 psia
 Vapor fraction:
 Total flow basis: Mole
 Total flow rate:
 Solvent:
 Reference Temperature
 Volume flow reference temperature:
 Component concentration reference temperature:
 Composition

Component	Value
TOLUENE	200
METHY-DI	200
PHENOL	
Total	400

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Models

Simulation 1 - Aspen Plus V8.8 - aspenONE

Capital: ___ USD Utilities: ___ USD/Year Energy Savings: ___ MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet: FEED (MATERIAL) B1 (RadFrac)

Configuration

Setup options

Calculation type: Equilibrium
 Number of stages: 22
 Condenser: Total
 Reboiler: Kettle
 Valid phases: Vapor-Liquid
 Convergence: Standard

Operating specifications

Distillate rate: Mole 200 lbmol/hr
 Reflux ratio: Mole 8
 Free water reflux ratio: 0

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Models

Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Model Summary Input Stream Analysis Heat Exchanger Pressure Relief
Stream Summary History Sensitivity Azeotrope Search PRD Rating
Utility Costs Report Data Fit Distillation Synthesis Flare System
Summary Analysis Safety Analysis

Simulation Capital: ___USD Utilities: ___USD/Year Energy Savings: ___MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

All Items
Setup
Property Sets
Analysis
Flowsheet
Streams
FEED
Input
Results
EO Variables
Stream Results (Cur
MCHTOP
BOTTOM
Blocks
B1
Specifications
Configuration
Sizing and Rating
Rate-Based Models
Analysis
Convergence
Dynamics
EO Modeling
Results

Properties
Simulation
Safety Analysis
Energy Analysis

Main Flowsheet FEED (MATERIAL) B1 (RadFrac)

Configuration Streams Pressure Condenser Reboiler 3-Phase Information

View Top / Bottom

-Top stage / Condenser pressure
Stage 1 / Condenser pressure 16 psia

-Stage 2 pressure (optional)
Stage 2 pressure psia
Condenser pressure drop psi

-Pressure drop for rest of column (optional)
Stage pressure drop psi
Column pressure drop psi

Model Palette
Mixer/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Models
Material DSTWU Dist RadFrac Extract MultiFrac SCFrac PetroFrac ConSep BatchSep

Required Input Complete Check Status

Search the web and Windows

Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Model Summary Input Stream Analysis Heat Exchanger Pressure Relief
Stream Summary History Sensitivity Azeotrope Search PRD Rating
Utility Costs Report Data Fit Distillation Synthesis Flare System
Summary Analysis Safety Analysis

Simulation Capital: ___USD Utilities: ___USD/Year Energy Savings: ___MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

All Items
Setup
Property Sets
Analysis
Flowsheet
Streams
FEED
Input
Results
EO Variables
Stream Results (Cur
MCHTOP
BOTTOM
Blocks
B1
Specifications
Configuration
Sizing and Rating
Rate-Based Models
Analysis
Convergence
Dynamics
EO Modeling
Results

Properties
Simulation
Safety Analysis
Energy Analysis

Main Flowsheet FEED (MATERIAL) B1 (RadFrac)

Configuration Streams Pressure Condenser Reboiler 3-Phase Information

Condenser specification
Temperature F
Distillate vapor fraction Mole 0

Subcooling specification
Subcooled temperature F
Both reflux and liquid distillate are subcooled
Only reflux is subcooled

Utility specification
Utility

Model Palette
Mixer/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Models
Material DSTWU Dist RadFrac Extract MultiFrac SCFrac PetroFrac ConSep BatchSep

Required Input Complete Check Status

Search the web and Windows

Simulation 1 - Aspen Plus V8.8 - aspenONE

Capital: ___ USD Utilities: ___ USD/Year Energy Savings: ___ MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet: FEED (MATERIAL) > B1 (RadFrac)

Configuration | Streams | Pressure | **Reboiler** | 3-Phase | Information

Thermisiphon reboiler options

- Specify reboiler flow rate
- Specify reboiler outlet condition
- Specify both flow and outlet condition

Flow rate: Mole 1.00 lbmol/hr

Outlet condition: Temperature

Optional

- Reboiler pressure: 16 psia
- Reboiler return feed convention: Above-Stage
- Utility: []

Reboiler configurations

Model Palette: Material, DSTWU, Dist, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, ConSep, BatchSep

Simulation 1 - Aspen Plus V8.8 - aspenONE

Capital: ___ USD Utilities: ___ USD/Year Energy Savings: ___ MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet: FEED (MATERIAL) > B1 (RadFrac)

Configuration | Streams | **Pressure** | Condenser | Reboiler | 3-Phase | Information

View: Top / Bottom

Top stage / Condenser pressure: 16 psia

Stage 1 / Condenser pressure: 16 psia

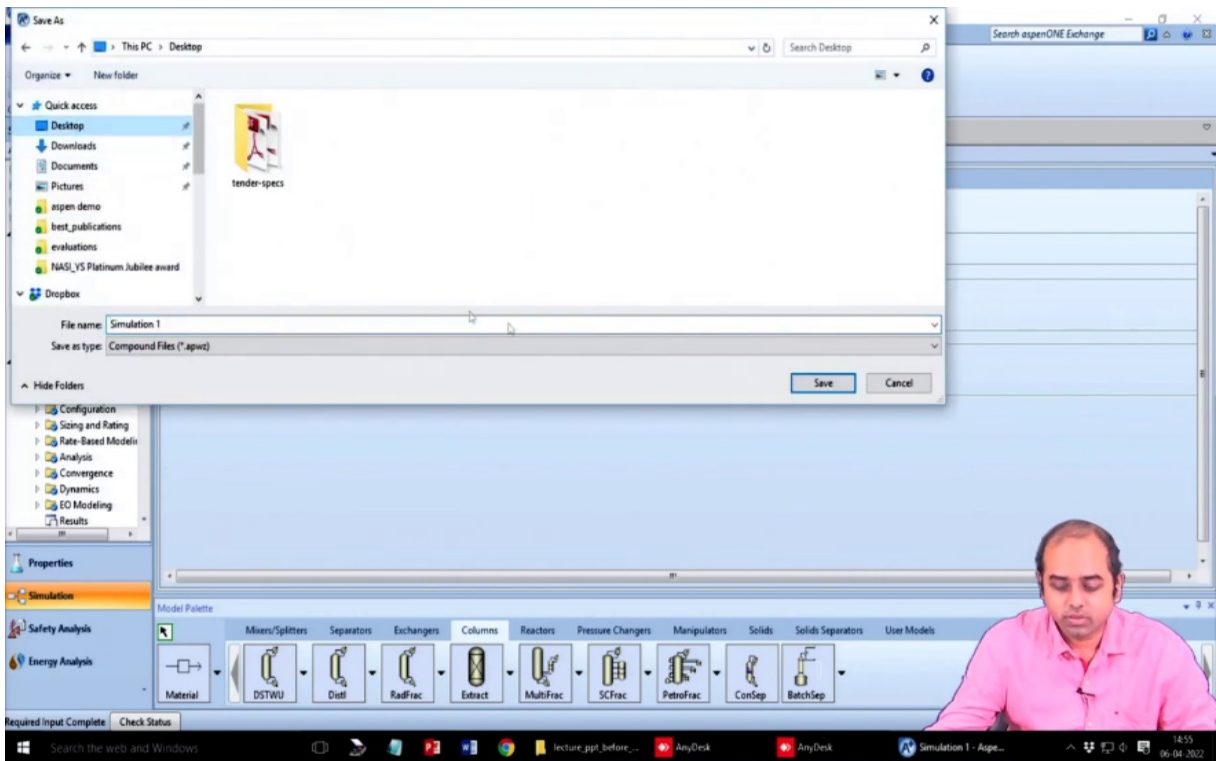
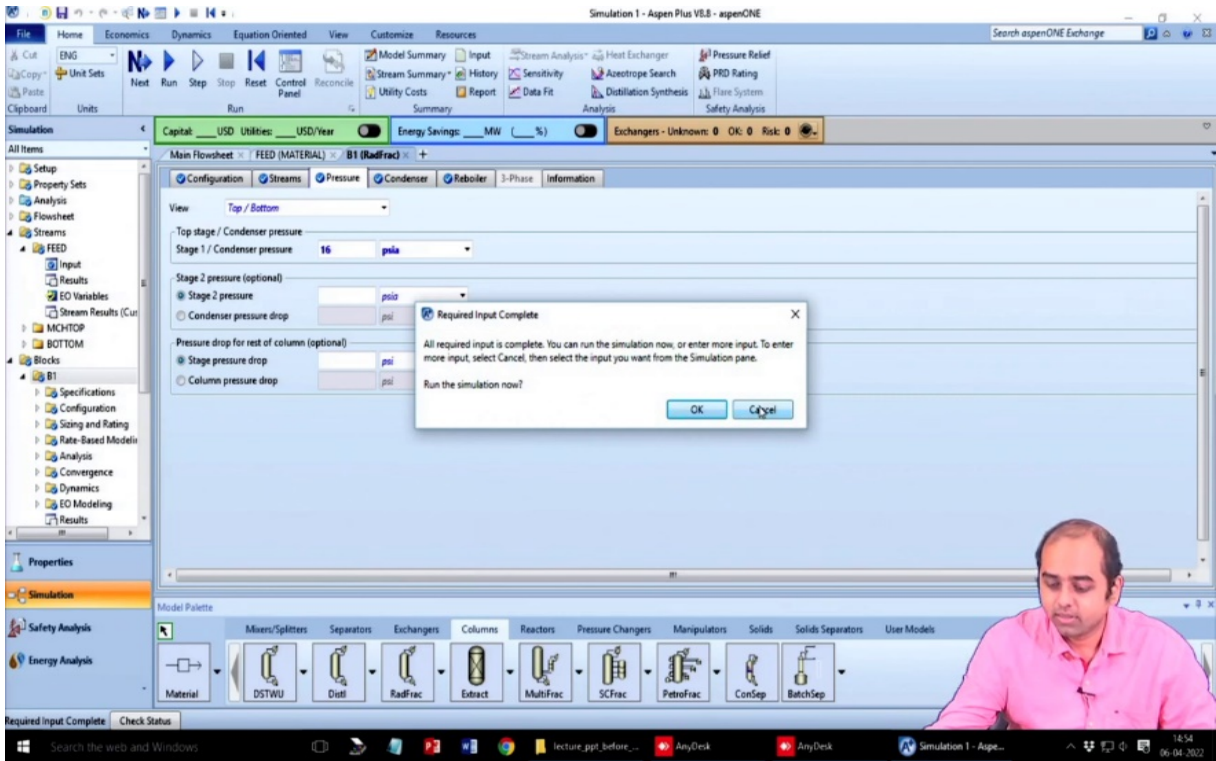
Stage 2 pressure (optional)

- Stage 2 pressure
- Condenser pressure drop

Pressure drop for rest of column (optional)

- Stage pressure drop
- Column pressure drop

Model Palette: Material, DSTWU, Dist, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, ConSep, BatchSep



Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

Capital: USD Utilities: USD/Year Energy Savings: MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

Main flowsheet: FEED (MATERIAL) × B1 (RadFrac) × MCHTOP (MATERIAL) - Results

Display Streams: Format FULL Stream Table

Material	MCHTOP	BOTTOM
Substream: MIXED		
Mole Flow lbmol/hr		
TOLUENE	34.3572	165.643
METHY-01	165.643	34.3572
PHENOL	0	0
Total Flow lbmol/hr	200	200
Total Flow lb/hr	19429.9	18635.9
Total Flow cuft/hr	439.281	391.069
Temperature F	219.171	230.065
Pressure psia	16	16
Vapor Frac	0	0
Liquid Frac	1	1
Solid Frac	0	0
Enthalpy Btu/lbmol	-59921.8	-3119.91
Enthalpy Btu/lb	-616.801	-33.4828

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Models

Results Available Check Status

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

Capital: USD Utilities: USD/Year Energy Savings: MW (%) Exchangers - Unknown: 0 OK: 0 Risk: 0

Main flowsheet: FEED (MATERIAL) × B1 (RadFrac) × MCHTOP (MATERIAL) - Results × B1 (RadFrac) - Profiles

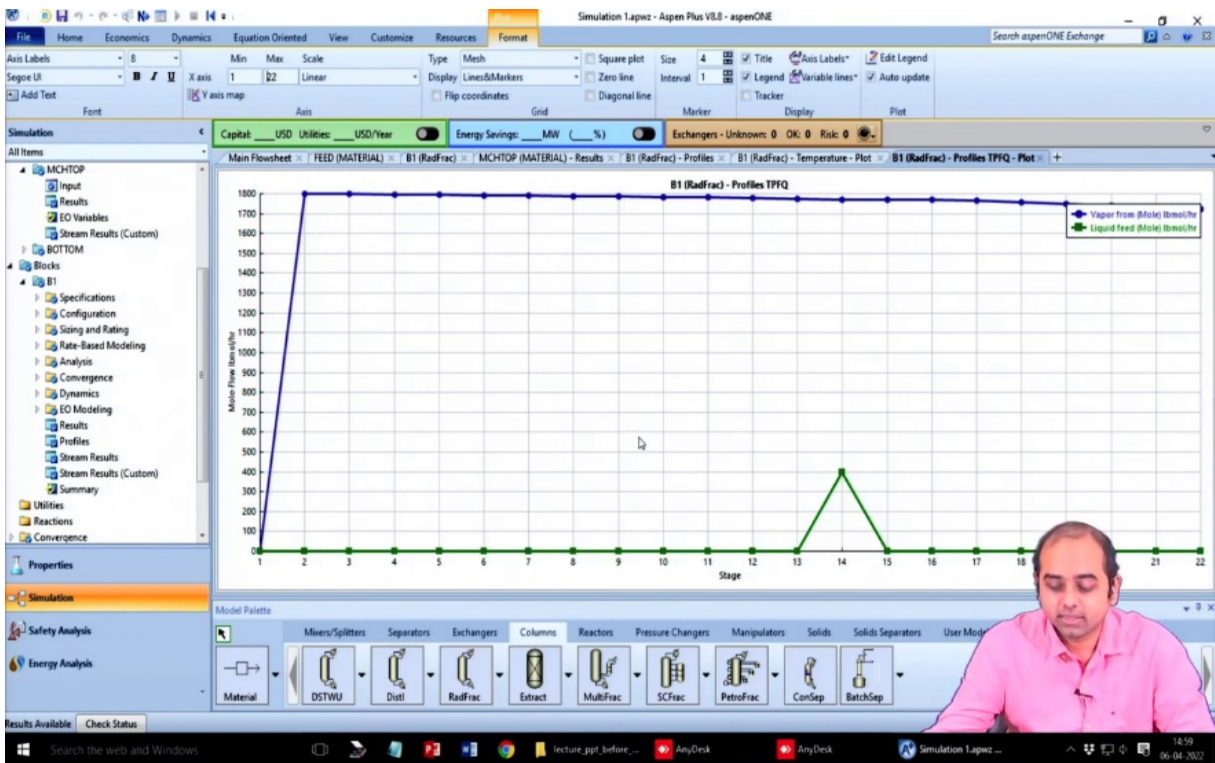
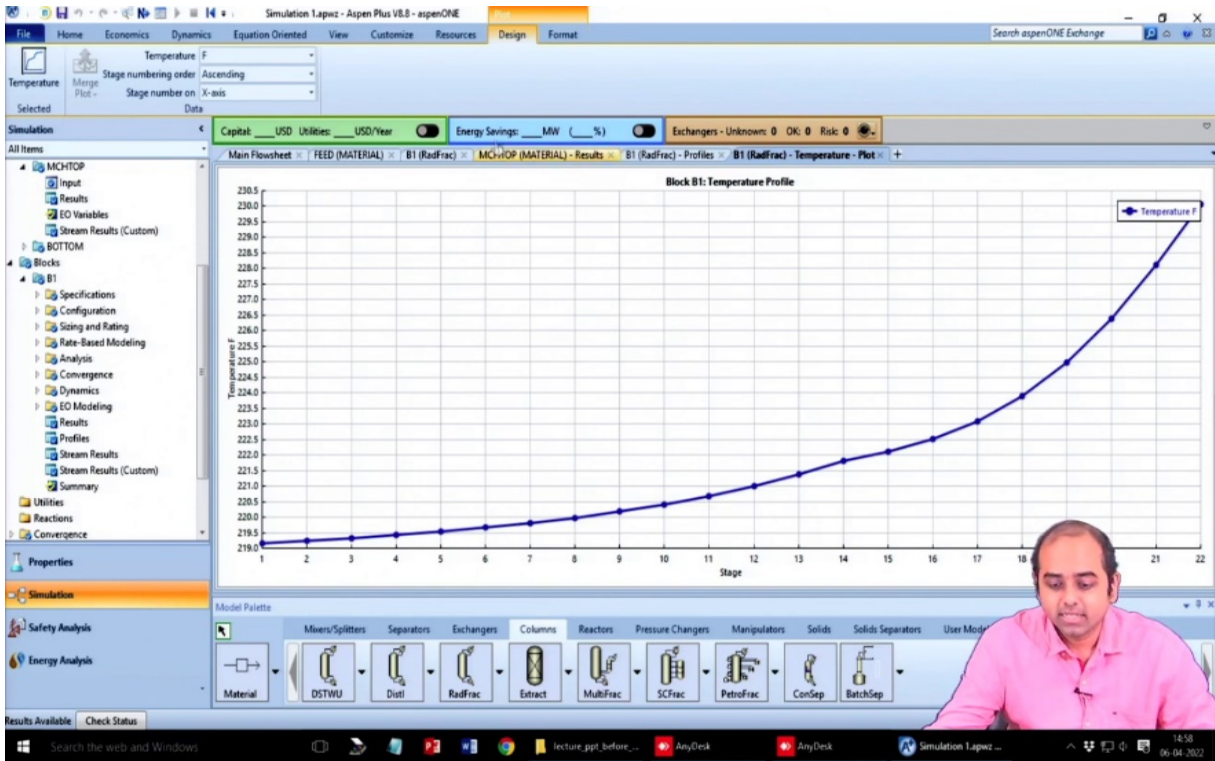
View: Basis Mole

Temperature: Stage or segment temperature vs. stage or segment number.

Stage	Temperature	Pressure	Heat duty	Liquid from (Mole)	Vapor from (Mole)	Liquid feed (Mole)	Vapor feed (Mole)	Mixed feed (Mole)	Liquid product (Mole)	Vapor product (Mole)	Liquid enthalpy	Vapor enthalpy	Liquid flow (Mole)	Vapor flow (Mole)
F	psia	Btu/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	Btu/lbmol	Btu/lbmol	lbmol/hr	lbmol/hr
1	219.171	16	-2.41668e+...	1800	0	0	0	0	200	0	-59921.8	-47541.4	1600	0
2	219.247	16	0	1596.5	1800	0	0	0	0	0	-58718.1	-46495.8	1596.5	1800
3	219.332	16	0	1596.94	1796.5	0	0	0	0	0	-57463.2	-45414.7	1596.94	1796.5
4	219.43	16	0	1595.26	1796.94	0	0	0	0	0	-56144.5	-44287.7	1595.26	1796.94
5	219.54	16	0	1593.45	1795.26	0	0	0	0	0	-54748.5	-43103.5	1593.45	1795.26
6	219.668	16	0	1591.48	1793.45	0	0	0	0	0	-53260.2	-41850	1591.48	1793.45
7	219.814	16	0	1589.33	1791.48	0	0	0	0	0	-51663.5	-40513.6	1589.33	1791.48
8	219.984	16	0	1587.07	1789.33	0	0	0	0	0	-49940.9	-39080.1	1587.07	1789.33
9	220.182	16	0	1584.39	1787.07	0	0	0	0	0	-48073.8	-37533.6	1584.39	1787.07
10	220.414	16	0	1581.48	1784.39	0	0	0	0	0	-46043.9	-35857.9	1581.48	1784.39
11	220.685	16	0	1578.29	1781.48	0	0	0	0	0	-43833.9	-34036.2	1578.29	1781.48
12	221.004	16	0	1574.78	1778.29	0	0	0	0	0	-41429.8	-32088.5	1574.78	1778.29
13	221.377	16	0	1570.92	1774.78	0	0	0	0	0	-38824.7	-30000.2	1570.92	1774.78

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Models

Results Available Check Status



Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

CapEx: USD Utilities: USD/Year Energy Savings: MW (%) Exchanges: Unknown 0 OK: 0 Risk: 0

Main FlowSheet: FEED (MATERIAL) | B1 (RadFrac) | MCHTOP (MATERIAL) - Results | B1 (RadFrac) - Profiles | B1 (RadFrac) - Temperature - Plot

TFPQ Compositions K-Values Hydraulics Reactions Efficiencies Properties Key Components Thermal Analysis Hydraulic Analysis Bubble Dew Points

View All Basis Mole

Stage	Temperature	Pressure	Heat duty	Liquid from (Mole)	Vapor from (Mole)	Liquid feed (Mole)	Vapor feed (Mole)	Mixed feed (Mole)	Liquid product (Mole)	Vapor product (Mole)	Liquid enthalpy	Vapor enthalpy	Liquid flow (Mole)	Vapor flow (Mole)
F	psia	Btu/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	Btu/lbmol	Btu/lbmol	lbmol/hr	lbmol/hr
1	219.171	16	-2.41668e+06	1800	0	0	0	0	200	0	-59921.8	-47541.4	1600	0
2	219.247	16	0	1598.5	1800	0	0	0	0	0	-58718.1	-46495.8	1598.5	1800
3	219.332	16	0	1596.94	1798.5	0	0	0	0	0	-57463.2	-45414.7	1596.94	1798.5
4	219.43	16	0	1595.26	1796.94	0	0	0	0	0	-56144.5	-44287.7	1595.26	1796.94
5	219.54	16	0	1593.45	1795.26	0	0	0	0	0	-54748.5	-43103.5	1593.45	1795.26
6	219.668	16	0	1591.48	1793.45	0	0	0	0	0	-53260.2	-41850	1591.48	1793.45
7	219.814	16	0	1589.33	1791.48	0	0	0	0	0	-51663.5	-40513.6	1589.33	1791.48
8	219.984	16	0	1587.07	1789.33	0	0	0	0	0	-49940.9	-39000.1	1587.07	1789.33
9	220.182	16	0	1584.39	1787.07	0	0	0	0	0	-48073.8	-37533.6	1584.39	1787.07
10	220.414	16	0	1581.48	1784.39	0	0	0	0	0	-46043.9	-35857.9	1581.48	1784.39
11	220.685	16	0	1578.29	1781.48	0	0	0	0	0	-43833.9	-34036.2	1578.29	1781.48
12	221.004	16	0	1574.78	1778.29	0	0	0	0	0	-41429.8	-32095.5	1574.78	1778.29
13	221.377	16	0	1570.92	1774.78	0	0	0	0	0	-38824.7	-30000.1	1570.92	1774.78

Model Palette: Material, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, ConSep, BatchSep

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

CapEx: USD Utilities: USD/Year Energy Savings: MW (%) Exchanges: Unknown 0 OK: 0 Risk: 0

B1 (RadFrac) - Stream Results: Main FlowSheet: FEED (MATERIAL) | B1 (RadFrac) | MCHTOP (MATERIAL) - Results | B1 (RadFrac) - Profiles | B1 (RadFrac) - Temperature - Plot | B1 (RadFrac) - Profiles TFPQ - Plot

TFPQ Compositions K-Values Hydraulics Reactions Efficiencies Properties Key Components Thermal Analysis Hydraulic Analysis Bubble Dew Points

View All Basis Mole

Stage	Temperature	Pressure	Heat duty	Liquid from (Mole)	Vapor from (Mole)	Liquid feed (Mole)	Vapor feed (Mole)	Mixed feed (Mole)	Liquid product (Mole)	Vapor product (Mole)	Liquid enthalpy	Vapor enthalpy	Liquid flow (Mole)	Vapor flow (Mole)
F	psia	Btu/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	lbmol/hr	Btu/lbmol	Btu/lbmol	lbmol/hr	lbmol/hr
1	219.171	16	-2.41668e+06	1800	0	0	0	0	200	0	-59921.8	-47541.4	1600	0
2	219.247	16	0	1598.5	1800	0	0	0	0	0	-58718.1	-46495.8	1598.5	1800
3	219.332	16	0	1596.94	1798.5	0	0	0	0	0	-57463.2	-45414.7	1596.94	1798.5
4	219.43	16	0	1595.26	1796.94	0	0	0	0	0	-56144.5	-44287.7	1595.26	1796.94
5	219.54	16	0	1593.45	1795.26	0	0	0	0	0	-54748.5	-43103.5	1593.45	1795.26
6	219.668	16	0	1591.48	1793.45	0	0	0	0	0	-53260.2	-41850	1591.48	1793.45
7	219.814	16	0	1589.33	1791.48	0	0	0	0	0	-51663.5	-40513.6	1589.33	1791.48
8	219.984	16	0	1587.07	1789.33	0	0	0	0	0	-49940.9	-39000.1	1587.07	1789.33
9	220.182	16	0	1584.39	1787.07	0	0	0	0	0	-48073.8	-37533.6	1584.39	1787.07
10	220.414	16	0	1581.48	1784.39	0	0	0	0	0	-46043.9	-35857.9	1581.48	1784.39
11	220.685	16	0	1578.29	1781.48	0	0	0	0	0	-43833.9	-34036.2	1578.29	1781.48
12	221.004	16	0	1574.78	1778.29	0	0	0	0	0	-41429.8	-32095.5	1574.78	1778.29
13	221.377	16	0	1570.92	1774.78	0	0	0	0	0	-38824.7	-30000.1	1570.92	1774.78

Model Palette: Material, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, ConSep, BatchSep

Stage	TOLUENE	METHY-01
8	0.274543	0.725457
9	0.295593	0.704407
10	0.318541	0.681459
11	0.343599	0.656401
12	0.370945	0.629055
13	0.400681	0.599319
14	0.432784	0.567216
15	0.453294	0.546706
16	0.480509	0.519491
17	0.516082	0.483918
18	0.561458	0.438542
19	0.617154	0.382846
20	0.681759	0.318241
21	0.75114	0.24886
22	0.81898	0.18102

So, now let us go to the simulation block. So, I clicked on the simulation block already. Let me remove this and do it once again for you. So, I go to the columns, I choose the RadFrac, and I just click it here. So, click RadFrac, and then click. You can also drag it, but this is same only, and next I have to connect these streams. So, again, streams could be of several types. It could be material streams, which is the most common one.

It could also be a heat stream. If you want some heat and energy inputs to the system, or it could be also work stream. So, we select the material stream. Let us say, I mark this one as 1 and do a marking of the, all the streams. And this one, let me say, I write down as feed something like top. So, you have to be careful that I cannot use the reserve mean because these names are essentially the names of the different stream variables.

So, let me write MCHTOP, let us write BOTTOM. So, these are the different streams that we got. Now, it is time to specify the stream inputs, as well as the column inputs. So, if you double click on the streams, so this is the feed stream. Now, as part of the problem, it is said that in the feed, you are getting the methylcyclohexane as 200-pound moles per hour. Toluene is 200-pound moles per hour. And the temperature is 220 Fahrenheit. So, let us put the value. So, temperature is 220 pressure is 20 psia.

And then it asks that whether there are two options, either you can specify the mole fractions and specify a total flow rate, or you can also specify the individual component fluid. So, if you are specifying individual component fluid, total fluid, it not to be specified. So, let us say I specify toluene fluid as 200 and methylcyclohexane as 200. So, we will see automatically your total is done 400. So, this specification of the total flow rate is not required. So, this is the feed stream.

The outlet streams are something that will come as a part of the calculation. So, we need not to worry about that. Now, coming to the distillation column. So, then the distillation column first it first it talks about the number of stages about the condenser, boiler and specification of the distillate or the reflux, all those things. So, let us say the calculation type is equilibrium. And for the first case, let us fix the number of stages 22, condenser it asks for whether you want to go for total or whether you want to go for partial vapor partial, vapor liquids. Let us select total. Reboiler is by default. Kettle is the most recommended choice.

Now, it comes to the operating specifications. Like what is the distillate rate either you specify that or you specify that reflux ratio, you can also specify other things like reboiler duty, the boiler rate, the condenser duty, all those things can also be specified. So, any two properties should be specified. So, let us say, we specify these two properties. So, the reflux ratio is given in the problem as 8. And the distillate rate is mentioned as 200 moles per hour, pound moles per hour. So, we specify that as 200-pound moles per hour and the reflux ratio is 8.

So, after you write the number you press enter. So, that is like entered into the system and it will mark as bold. Next is the streams. So, in the streams it will ask like what is the feed stage? So, for the first problem, instead of varying trying to vary and see what is the effect, let us mark the feed stage as 14 and in the product stream, you will see that MCH top represents stage one. And the bottom stream represents 22. So, total 22 number of stages we have specified, then it asks for the pressure. So, now these two blocks are already, tabs are already clicked blue. So, next day it asks for the pressure.

So, it asks that what is the condenser pressure in the, or the stage one pressure? That is the minimum, the requirement that you need to specify. So, it is mentioned that the condenser pressure is 16 psia. And rest of this information is optional. If you go to the condenser, it will, it is already ticked blue. So, all the necessary specification is provided. For the case of the reboiler also, it is already ticked.

I mean, it is already marked in blue. So, already those specifications are provided in this case. So, now everything is blue. So, now you see the bottom of the software. There is a message, which says that the required input is complete. So, the mandatory or the minimum requirements needed for the problem to work is completed. So, once this is done, you have to initialize your run. So, the initialization step is. So, once the required input is done, the system is automatically initialized.

Now, that in the first case, since we have provided these values, it is not asking for initialization. Now, if you run it and then change some of the input, it will ask that the system or the simulation is not initialized properly. So, you need to re initializing it. So, for the first case, this will not be asked. A general practice is to save the simulation before we go for subsequent new analysis or running the system.

So, let us run it and then let us try to evaluate the results for the first case. So, if I click on run, within a few seconds, suddenly the results will be, it is marked as results are available. So, computation is completed. So, how do you check the results? So, now if you go to the main flow sheet, the results are available from clicking on the streams or the outlet streams. So, if you now select outlet streams, you will see that the values are already listed down or table it down.

So, for example, this is the top stream, and you will see that the top stream that toluene fluid is 34 and methylcyclohexane is 165. Total is of course 200 that has to satisfy Temperature is also specified for Fahrenheit is 219 of the top stream. And the rest of the energy parameters

are also specified, you can also list down the other bottom stream here. So, these are the bottom stream specifications. And you see on the bottom side, the quantity of toluene is more compared to methylcyclohexane.

So, you can also try to make a plot of these profiles across the different stages that is also possible. So, how do you look into that? If you go to the main flow sheet, and if in the left-hand side, if you click on the block results. So, please see that on the left-hand side, you have the blocks marked as B1, because we had only one block or one-unit operation block. So, after the calculation is done here, there are options of the stream results and the profiles.

So, if you click on this profile, it will give you the stage wise composition. So, the first column represents the stage number, and you will see that across each of the stages. How does the temperature change? So, naturally toluene is the more heavier compound compared to cyclohexane. And as a result, you see that the bottom temperature is more than the top temperature. So, this is how the temperature changes.

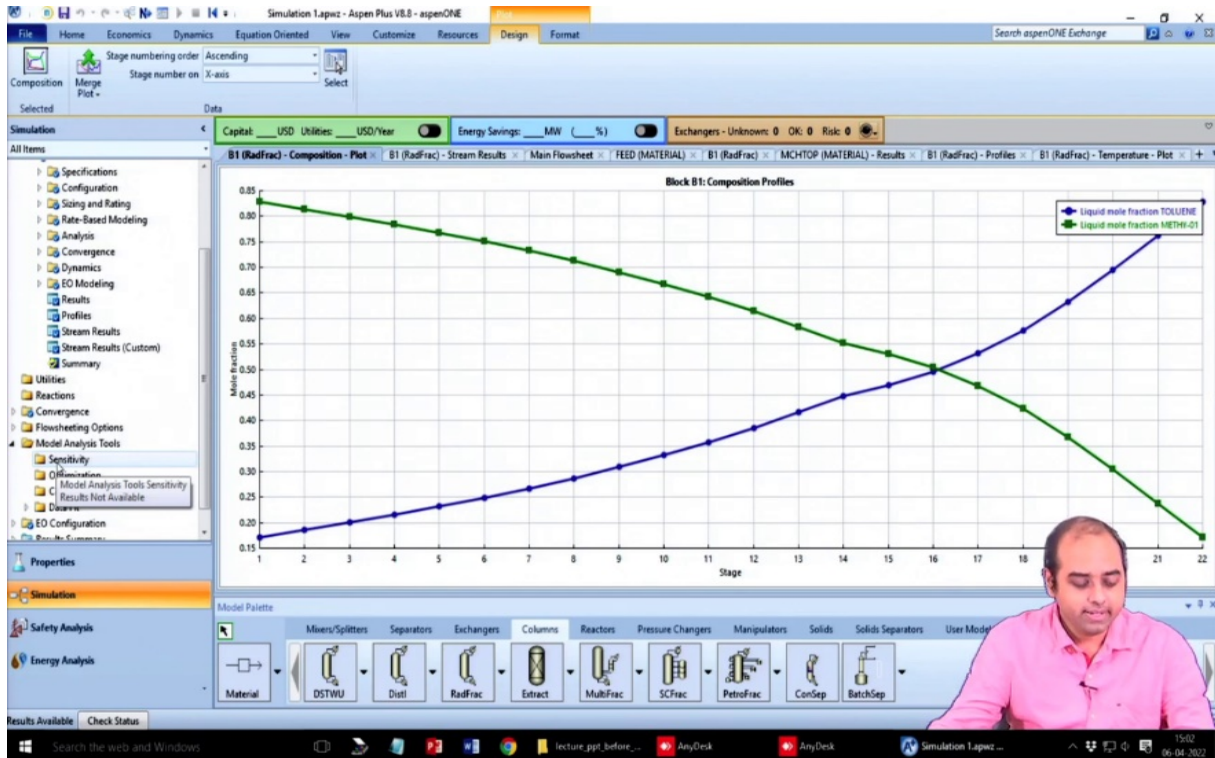
Similarly, you have these other properties, for example, that there is liquid rates and the vapor flow rates in each of the stages, all these information are provided to you. So, everything is calculated based on the mole fractions. So, you can essentially make a, a plot let us say, so I can make a plot of the temperature stage and the segment temperature. If I click on that, it will show that how the temperature changes across the stages.

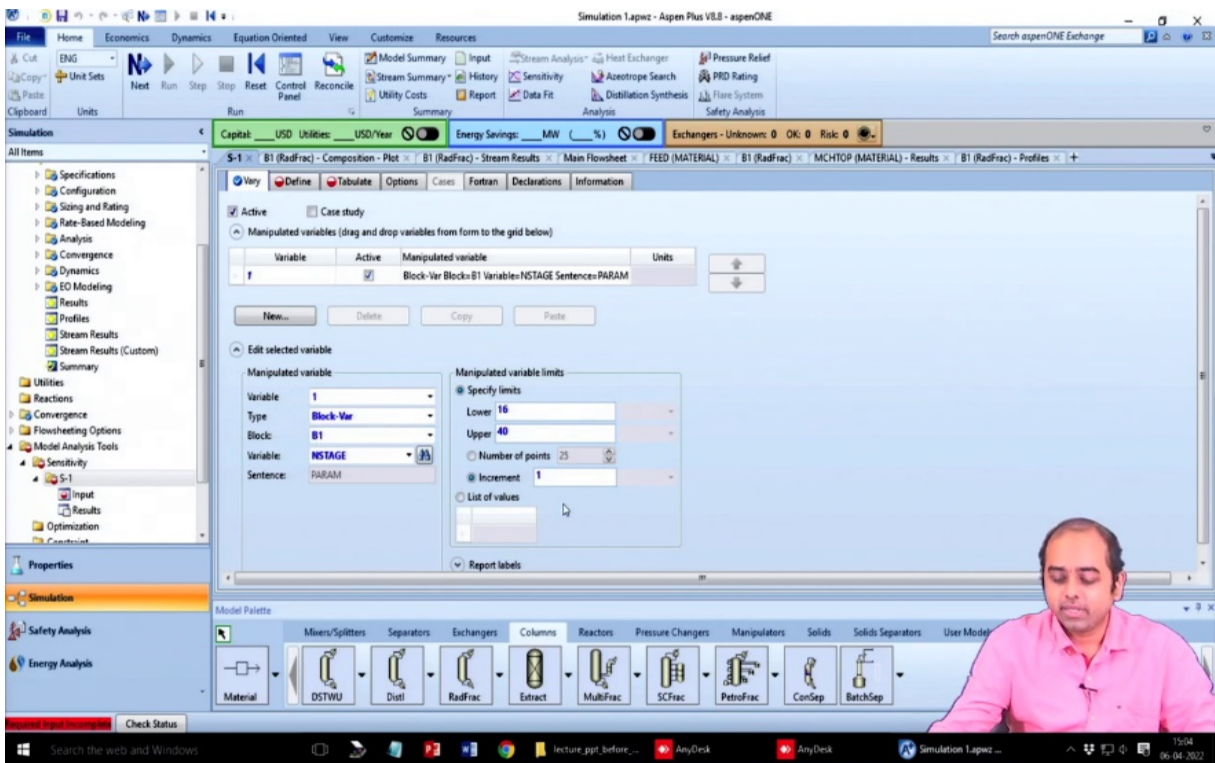
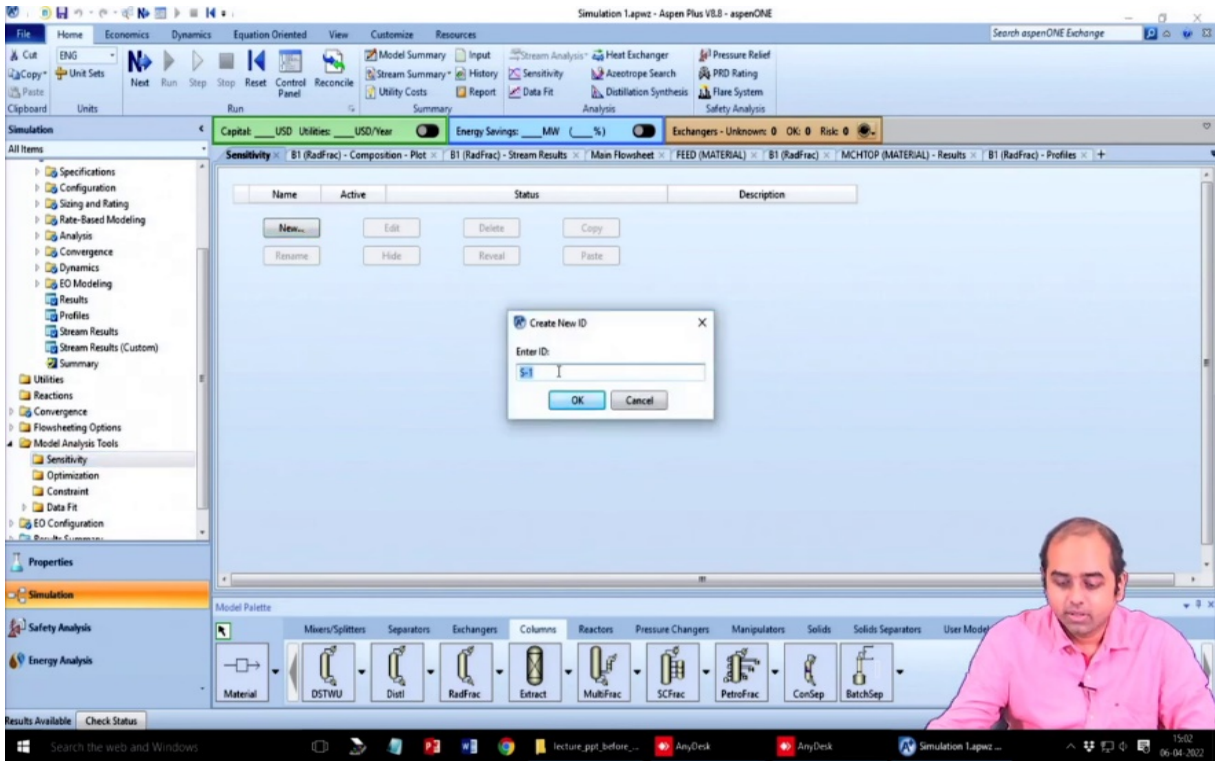
Similarly, I can also work on the, on the profiles and I can see if I want to plot the liquid or the vapor across different stages. That is also possible. So, stage 14 is the feed stage. That is where you will see that the mole flow rate is 200 on the liquid feed and rest is mostly vapor in each of the stages. You can also look into this stream mole fractions. So, I am just trying to get that. Yes. So, in this profile, you will see that there are different tabs. The first one is the tabs, which represent the temperature.

Most of the vapor liquid flow rates, there is the next small tab known as a composition. And here, if you see that the compositions, liquid phase compositions of the toluene and methylcyclohexane across each of the trays is mentioned. So, this methylcyclohexane is more enriched at the top and is what you are also seeing. The top fraction cyclone is almost 83 percent and we realize that beyond that it is not actually thermodynamically possible to improve its more fraction because it almost forms as azeotrope.

And you see in the last, first few stages, the change in the mole fraction is very, very small. It is only beyond, this fifth or sixth tray, you start to see a big changes in the mole fractions, and the last stage, the toluene mole fraction is higher compared to the methylcyclohexane. So, this is also something that we can plot composition. So, this is the tray wise composition of the toluene and the methylcyclohexane. So, this is all about analysis depending on this, case of the, this separating of the two components.

(Refer Slide Time: 39:39)





Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Simulation: Capital USD Utilities USD/Year Energy Savings MW Exchanges - Unknown 0 OK 0 Risk 0

S-1 B1 (RadFrac) - Composition - Plot B1 (RadFrac) - Stream Results Main Flowsheet FEED (MATERIAL) B1 (RadFrac) MCHTOP (MATERIAL) - Results B1 (RadFrac) - Profiles

Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition

Enter variable name: MCHDIST

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Model

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Simulation: Capital USD Utilities USD/Year Energy Savings MW Exchanges - Unknown 0 OK 0 Risk 0

S-1 B1 (RadFrac) - Composition - Plot B1 (RadFrac) - Stream Results Main Flowsheet FEED (MATERIAL) B1 (RadFrac) MCHTOP (MATERIAL) - Results B1 (RadFrac) - Profiles

Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
MCHDIST	Mole-Frac Stream=MCHTOP Substream=MIXED Component=METHY-01

Edit selected variable

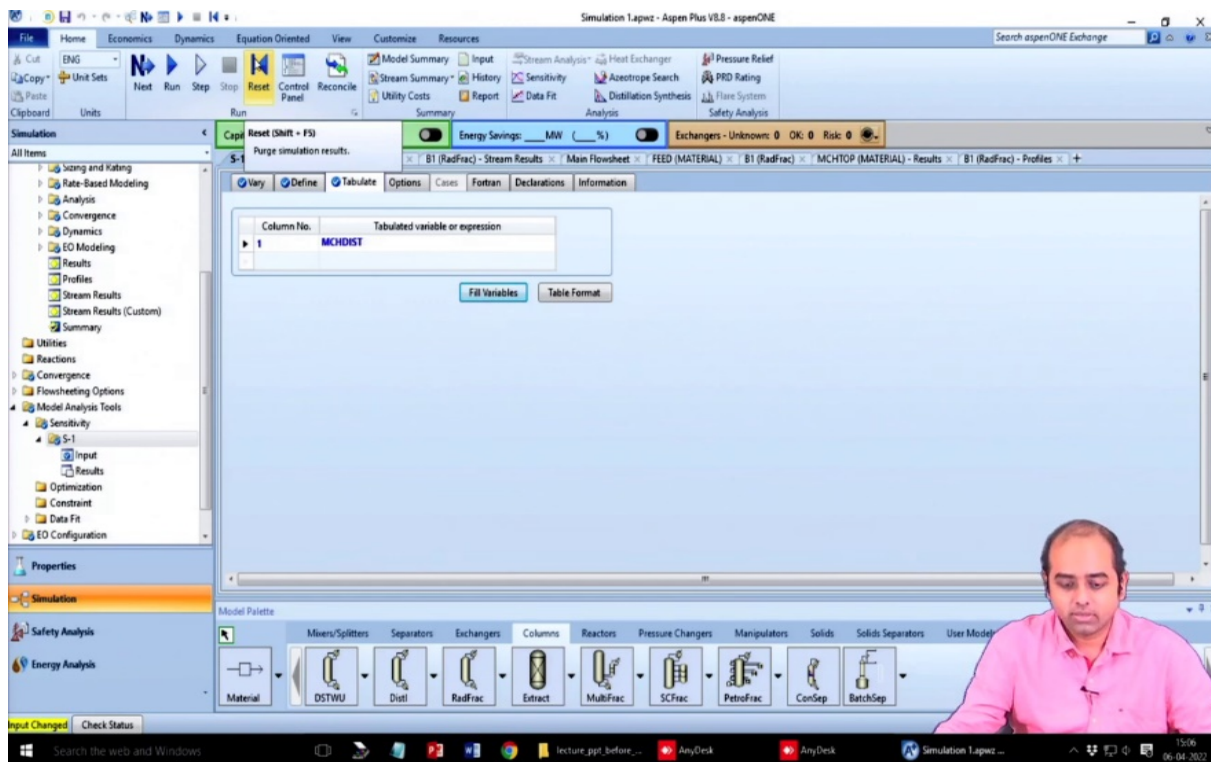
Variable: MCHDIST

Category: Streams

Reference:

- Type: Mole-Frac
- Stream: MCHTOP
- Substream: MIXED
- Component: METHY-01

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Model



Next thing I wanted to show is about the sensitivity. Like, so let us go into the sensitivity block. So, what is sensitivity? Essentially, sensitivity means if I want to, or if I want to alter one particular variable in my system and see what is the effect in the final solution? So, it is like a loop, I put the variation of one of my variables. I have to specify all the range and et cetera.

And also, I have to specify that what is the final output variable that I want to track. And accordingly, then based on the variation of my manipulative variable, how does the output variable, which I have defined changes? So, that is what the sensitivity, so let us say the sensitivity. I will try to work here this model analysis tools, and there is option called sensitivity. So, after you have run the base case simulation, the next step is to work out or to try to see that with the sense that, how things, this sensitivity how we can vary.

So, I click on the sensitivity, ask for the variable name. So, let us say, I write it as you know, S 1 and then it will ask that what is the variable that you want to vary? So, I have to choose that variable. So, first let me decide is variable number 1 and type. Here, you have to choose it very carefully. So, these type means that what is the category of the variable? So, depending on the type, then it will, subcategorize, it will have the sub classifications.

So, let us say, in this case, I want to, instead of fixing 22 columns, I want to vary, sorry, not 22 columns, 22 stages. I want to vary. Let, I want to vary from 20 to 50 and see that

increasing the number of say, let us 20 to 40. I want to vary all it from 15 or 16 to 40 I want to vary and see that whether increasing the number of stages does help in improving the enrichment of the methylcyclohexane in the distillate.

So, the manipulated variable is essentially the number of stages. So, I select that as the block variable, and then after it will at which block, so is only one block B1, and now it will at what is the variable in the block or in this block B1 one that you want to change. So, it is like hierarchical category. So, here you will see that there is a lot of variables, which is part of the calculations.

You can also identify them by the names, NSTAGE represents the number of theoretical stages, which includes the condenser as well as the reboiler. So, that is the variable I want to vary now, what is the limits of the variation that is also, I have to specify lower limit as well as the upper limit. So, let us say one to vary from 16 to 40 and increment of 1. There is no point, sorry, increment of one. There is no fractional stage possible. So, I put increment as 1. So, this is how my manipulative variable is defined.

Next, I have to specify the output variable, let us say the output variable I write MCH this top distillation. And here it will ask that in this variable, what you want to I mean, what is the variable that you want to track? So, let us say track streams and I select type as the mole fraction. So, it is the mole fraction. It will ask for stream, MCH top it is again hierarchical. Stream is mixed. So, component with more fraction of what? Mole fraction of methylcyclohexane that I want to study.

So, this completes the definition of the output variable that I want to track. Next is the tabulate option. So, in the tabulate option if you just click on this, fill the variables, it will automatically fill that it will have one column where it will list down the values of the top distillate based on the variation of my manipulated variable, which is the number of stages in this case. Now, you see that at the bottom, it is written input is changed. So, if the input is changed, you need to click on this reset, and then rerun your simulation.

So, reset it again, resetting the simulation and initializing it properly. So, now all the analysis is done. I mean, sorry, the sensitivity is selected and now you have to rerun your simulation. Reinitialize. So, now all results will be cleared and sequence will be started from the beginning and next you have to do this run. So, if I now click on this run, the calculation says that some results are coming, but with error. So, let us see.

(Refer Slide Time: 45:23)

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

Simulation Errors

Your simulation has completed with errors. Results are present.

Display Run-Status results form
 Enter Equation Oriented input
 Synchronize Equation Oriented models

OK Cancel

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

Run Status

Convergence status
Block calculations were completed normally

Property status
Property calculations were completed normally

Aspen Plus messages:
** ERROR WHILE EXECUTING SENSITIVITY BLOCK: 'S-1'
SOME RIGS COMPLETED WITH ERRORS.

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Simulation: Capital USD Utilities USD/Year Energy Savings MW Exchanges - Unknown 0 OK 0 Risk 0

Model Analysis Tools: S-1 Input

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
1	<input checked="" type="checkbox"/>	Block-Var Block=B1 Variable=NSTAGE Sentence=PARAM	

Reinitialize dialog options:

- Simulation
- Number of points: 25
- Increment: 1
- List of values

Model Palette: Material, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, ConSep, BatchSep

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Simulation: Capital USD Utilities USD/Year Energy Savings MW Exchanges - Unknown 0 OK 0 Risk 0

Model Analysis Tools: S-1 Input

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
1	<input checked="" type="checkbox"/>	Block-Var Block=B1 Variable=NSTAGE Sentence=PARAM	

Aspen Plus dialog message:

Reinitialize Simulation purges all results and moves to the start of the sequence

Model Palette: Material, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, ConSep, BatchSep

The image displays two screenshots of the Aspen Plus V8.8 software interface, showing a sensitivity analysis table. The table lists 14 rows with 'Status' as 'OK' and 'VARY 1' as 'B1 PARAM NSTAGE'. The 'MCHDIST' values range from 0.787171 to 0.837406. The interface includes a menu bar, a toolbar, a simulation summary, and a model palette.

Row/Case	Status	VARY 1 B1 PARAM NSTAGE	MCHDIST
1	OK	16	0.787171
2	OK	17	0.796708
3	OK	18	0.807775
4	OK	19	0.814916
5	OK	20	0.820507
6	OK	21	0.824909
7	OK	22	0.828282
8	OK	23	0.830909
9	OK	24	0.832875
10	OK	25	0.834373
11	OK	26	0.835499
12	OK	27	0.836334
13	OK	28	0.836981
14	OK	29	0.837406

See, there are some errors. So, the error that it is showing in the sensitivity block is because of the fact in the base case of the this this column, we have specified the number of stages as 22, but in the run sensitivity analysis, we are trying to vary the number of stages from 16 to 40. So, in the case of sensitivity, this cannot be done because whatever, the number of stages that is specifying the base case in the sensitivity, it cannot exceed the base case value.

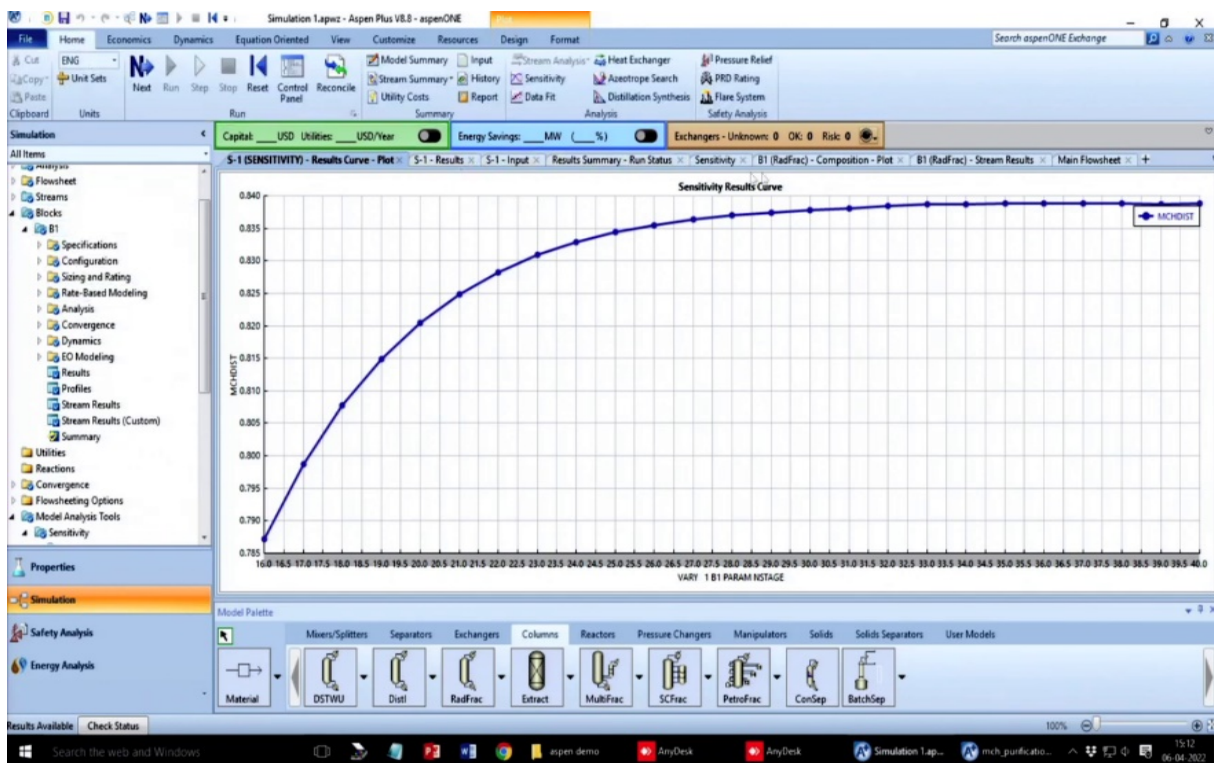
So, for the biggest case, you have to consider the highest value of what you are trying to alter or manipulate in the sensitivity. So, in this case, the total number has to be 40 because that is up to the higher limit. That is what we are trying to calculate in the sensitivity. So, now the sensitivity values that we have are inputs from 20 to sorry, 16 to 40 is within the base case values. So, let us reset the simulation once again. So, that will, purge all the solutions and then run the simulation.

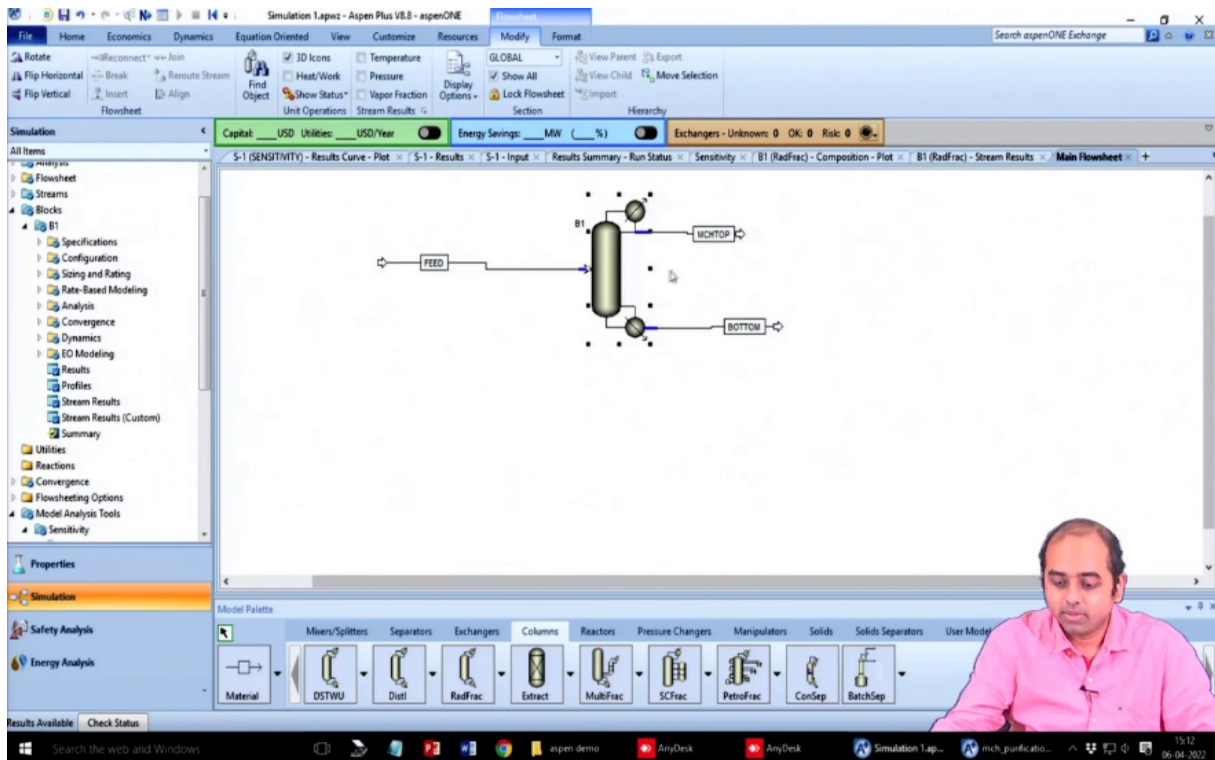
So, now in this case, you will see that the errors will not appear and you will see that there are no results it is already results are available. So, now if I click on the sensitivity results, I will see that, all are written as data. Because now everything is within the, this maximum value of the base case. So, if I try to plot this like stage versus composition, results curve, so, X axis is varying the number of stage Y axis is the MCH distillate.

So, according to the table, you will see that this is the plot that we can get. I hope it is visible to everyone. In the bottom X axis we have the number of stages and in the Y axis the distillate composition of the collection. And you see that even an increasing the number of stages, the concentration on the mole fraction does not increase significantly and suddenly not build above this thermodynamic limit. And this tells you that for azeotropes for azeotropic mixture, it is not sufficient only to increase the number of stage. You also need to add an entrainer. So, now let us look into this case where we have some phenol also into the system.

(Refer Slide Time: 48:15)

The screenshot shows the Aspen Plus V8.8 interface. A 'Results Curve' dialog box is open, allowing the user to select display options and curves to plot. The X-axis is set to 'VARY 1 B1 PARAM NSTAGE'. Under 'Select curve(s) to plot', 'MCHDIST' is selected. The background shows the main simulation window with various process icons in the Model Palette.





So, if you go to the again, simulation flow sheet flow sheet, let us go to the block and double click on that block. And in the streams, it asks that what is the feed? So, instead of one feed, we are planning to have another feed. So, first we have to add that stream and then we can have that in the feed or specify that as the phenol and the phenol flow rate. So, where is the simulation tab gone? Let us close so much of the tabs that are open already, main flow sheet.

(Refer Slide Time: 48:57)

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Simulation: Capital: USD Utilities: USD/Year Energy Savings: MW Exchanges - Unknown: 0 OK: 0 Risk: 0

B1 (RadFrac) - S-1 (SENSITIVITY) - Results Curve - Plot - S-1 - Results - S-1 - Input - Results Summary - Run Status - Sensitivity - B1 (RadFrac) - Composition - Plot - B1 (RadFrac) - Stream Results

Configuration Streams Pressure Condenser Reboiler 3-Phase Information

Feed streams

Name	Stage	Convention
FEED	14	Above-Stage

Product streams

Name	Stage	Phase	Basis	Flow	Units	Flow Ratio	Feed Specs
MCHTOP	1	Liquid	Mole		lbmol/hr		Feed basis
BOTTOM	40	Liquid	Mole		lbmol/hr		Feed basis

Pseudo streams

Name	Pseudo Stream Type	Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparound ID	Pumparound Conditions	Flow	Units
------	--------------------	-------	----------------	----------------	---------------------	---------------	-----------------------	------	-------

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Models

Results Available Check Status

15:13 06-04-2022

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Simulation: Capital: USD Utilities: USD/Year Energy Savings: MW Exchanges - Unknown: 0 OK: 0 Risk: 0

B1 (RadFrac) - B1 (RadFrac) - Stream Results - Main Flowsheet - FEED (MATERIAL) - MCHTOP (MATERIAL) - Results - B1 (RadFrac) - Profiles - B1 (RadFrac) - Temperature - Plot - B1 (RadFrac) - Profiles TPFQ - Plot

Configuration Streams Pressure Condenser Reboiler 3-Phase Information

Feed streams

Name	Stage	Convention
FEED	14	Above-Stage

Product streams

Name	Stage	Phase	Basis	Flow	Units	Flow Ratio	Feed Specs
MCHTOP	1	Liquid	Mole		lbmol/hr		Feed basis
BOTTOM	40	Liquid	Mole		lbmol/hr		Feed basis

Pseudo streams

Name	Pseudo Stream Type	Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparound ID	Pumparound Conditions	Flow	Units
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Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Models

Results Available Check Status

100% 15:13 06-04-2022

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Model Summary Input Stream Analysis Heat Exchanger Pressure Relief
 Stream Summary History Sensitivity Azeotrope Search PRD Rating
 Utility Costs Report Data Fit Distillation Synthesis Flare System
 Safety Analysis

Clipboard Units Run Next Run Step Stop Reset Control Panel Reconcile

Simulation Capital: USD Utilities: USD/Year Energy Savings: MW Exchanges - Unknown: 0 OK: 0 Risk: 0

All Items B1 (RadFrac) Main Flowsheet B1 (RadFrac) - Profiles B1 (RadFrac) - Temperature - Plot B1 (RadFrac) - Profiles TPFQ - Plot PHENOL (MATERIAL)

Setup Property Sets Analysis Flowsheet Streams BOTTOM FEED MCHTOP PHENOL Input Results EO Variables Stream Results (Custom) Blocks B1 Specifications Configuration Sizing and Rating Rate-Based Modeling Analysis Convergence Dynamics EO Modeling Results

Properties Simulation Safety Analysis Energy Analysis

Model Palette Mixers/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Model

Material DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac ConSep BatchSep

Specifications

Flash Type: Temperature Pressure

State variables: Temperature 220 F Pressure 20 psia Vapor fraction Total flow basis Mole Total flow rate Solvent

Reference Temperature: Volume flow reference temperature Component concentration reference temperature

Composition: Mole-Flow lbmol/hr

Component	Value
TOLUENE	
METHY-01	
PHENOL	1200
Total	1200

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources Modify Format

Rotate Reconnect 3D Icons Temperature GLOBAL Show All View Parent Export
 Flip Horizontal Break Reroute Stream Heat/Work Pressure Display Options Lock Flowsheet View Child Move Selection
 Flip Vertical Insert Align Show Status Vapor Fraction Stream Results Section Hierarchy

Simulation Capital: USD Utilities: USD/Year Energy Savings: MW Exchanges - Unknown: 0 OK: 0 Risk: 0

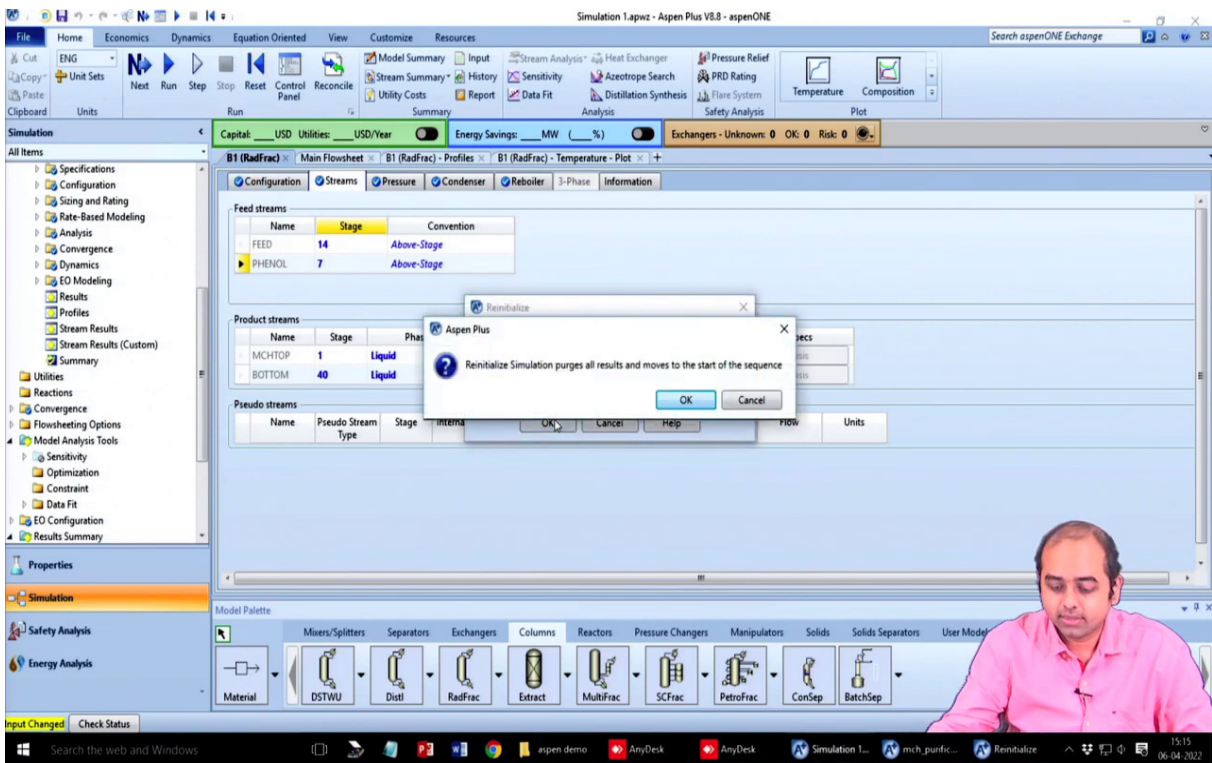
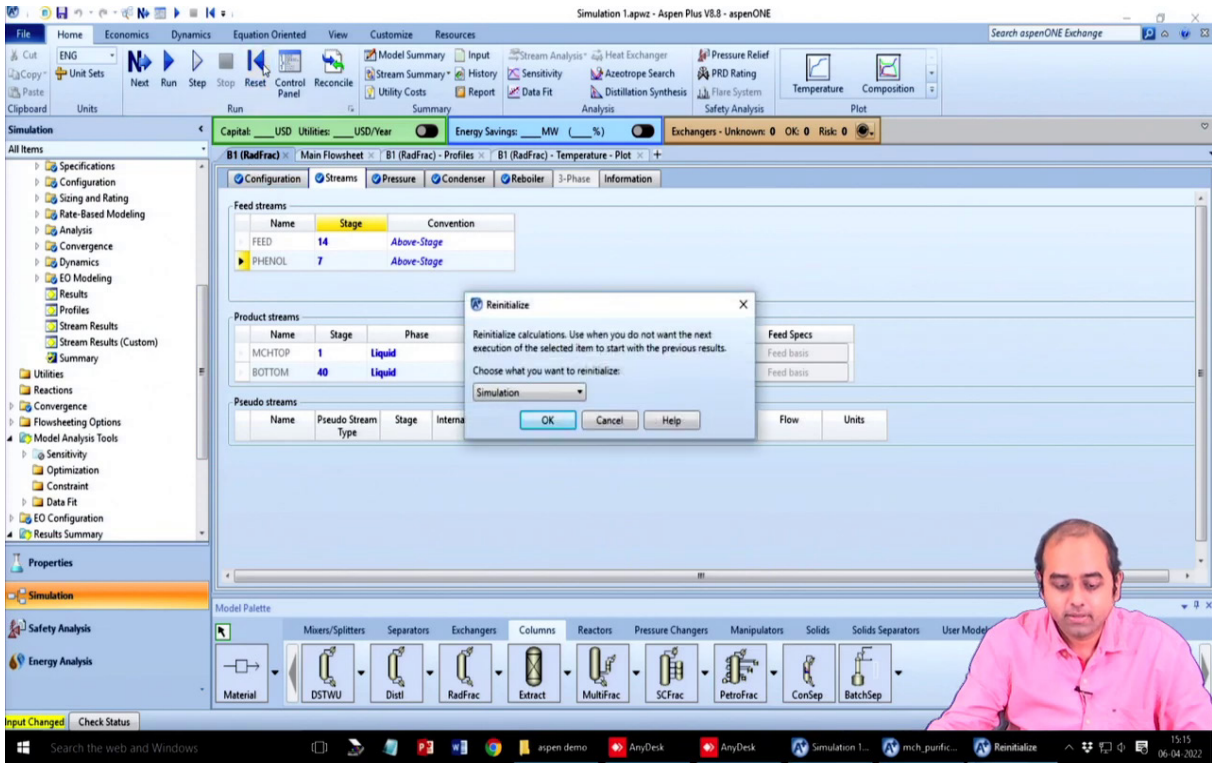
All Items B1 (RadFrac) Main Flowsheet B1 (RadFrac) - Profiles B1 (RadFrac) - Temperature - Plot B1 (RadFrac) - Profiles TPFQ - Plot

Setup Property Sets Analysis Flowsheet Streams BOTTOM FEED MCHTOP PHENOL Input Results EO Variables Stream Results (Custom) Blocks B1 Specifications Configuration Sizing and Rating Rate-Based Modeling Analysis Convergence Dynamics EO Modeling Results

Properties Simulation Safety Analysis Energy Analysis

Model Palette Mixers/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Model

Material DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac ConSep BatchSep



So, here, let us have another stream. And let us mark that as phenol. That is into the system. Now, if you, if you look carefully on this phenol stream, it will once again, ask that what is the temperature pressure, et cetera of this stream. So, we will specify that according to the problem and phenol, flow rate is also mentioned, sorry, temperature is 220 pressure is 20

psia. And the total flow rate. So, it is phenol. So, I will write total flow rate is given as 1200-pound moles per hour.

So, the rest are 0. So, we do not need to specify. Now, this stream specification is complete. So, next we have to go to this block and it will see that in the feed stream, it is asking for the stage numbers of these two feeds. So, one is the feed, the normal feed, which is a mixture of toluene and methylcyclohexane, next is the phenol. So, the phenol one is let say it is given and the problem as a seventh stage.

So, now it is time to rerun the calculations once again and see whether that the tray compositions have improved or at least the top composition is improved beyond 0.8 or what? We can disable the sensitivity for now, deactivate. So, we do not want the sensitivity. Now, it does first check with the phenol and then we will work on the sensitivity, reset and then run. So, now if you go to the results section or let us say the block here, I can see stage wise composition profiles.

So, now if you see that at the top stage, the previously, it was only up to 0.8 or 0.82. Now it has increased up to 0.98. So, further separation beyond the azeotropic limit is possible with the addition of the entrainer in this case, which is phenol. So, you can see clearly that the phenol composition is actually not too high in the top because phenol is the heavier one apart from methylcyclohexane. so that is why you see phenol is mostly at the bottom. So, it is not affecting much of the top distillate or the purity of the top distillate. So, we can quickly do a sensitivity of the phenol flow rate that how much phenol flow rate will be appropriate in this case to have a very high enrichment.

(Refer Slide Time: 52:06)

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

Capital: USD Utilities: USD/Year Energy Savings: MW (%) Exchanges - Unknown: 0 OK: 0 Risk: 0

B1 (RadFrac) - Results | Main Flowsheet | B1 (RadFrac) - Profiles | B1 (RadFrac) - Temperature - Plot

View: Liquid Basis: Mass

Stage	TOLUENE	METHY-01	PHENOL
1	0.0146156	0.984176	0.00120802
2	0.01453	0.982945	0.00252458
3	0.014473	0.980452	0.00507503
4	0.0144591	0.975206	0.0103351
5	0.0145211	0.962746	0.0227325
6	0.0147145	0.922073	0.0632125
7	0.0133121	0.540924	0.445763
8	0.0196154	0.534377	0.446008
9	0.0282272	0.525377	0.446396
10	0.0399787	0.513054	0.446968
11	0.0559675	0.496244	0.447788
12	0.0776065	0.473794	0.4486
13	0.106974	0.448006	0.44502
14	0.152994	0.457771	0.389235
15	0.153017	0.457746	0.389236

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Model

Results Available | Check Status

15:16 06-04-2022

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

Capital: USD Utilities: USD/Year Energy Savings: MW (%) Exchanges - Unknown: 0 OK: 0 Risk: 0

B1 (RadFrac) - Results | Main Flowsheet | Sensitivity | B1 (RadFrac) - Temperature - Plot

Name	Active	Status	Description
S-1	<input checked="" type="checkbox"/>	Inactive	

Buttons: New, Edit, Delete, Copy, Rename, Hide, Reveal, Paste

Create New ID dialog: Enter ID: S2

Model Palette: Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, User Model

Results Available | Check Status

15:16 06-04-2022

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

Model Summary Input Stream Analysis Heat Exchanger Pressure Relief
 Stream Summary History Sensitivity Azeotrope Search PRD Rating
 Utility Costs Report Data Fit Distillation Synthesis Flare System
 Summary Analysis Safety Analysis

Simulation Capital: USD Utilities: USD/Year Energy Savings: MW Exchanges - Unknown: 0 OK: 0 Risk: 0

All Items

- sizing and Rating
- Rate-Based Modeling
- Analysis
- Convergence
- Dynamics
- EO Modeling
- Results
- Profiles
- Stream Results
- Stream Results (Custom)
- Summary
- Utilities
- Reactions
- Convergence
- Flowsheeting Options
- Model Analysis Tools
 - Sensitivity
 - S-1
 - S-2
 - Input
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 - Optimization
 - Constraint

Properties

Simulation

Safety Analysis

Energy Analysis

Model Palette

Mixers/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Model

Material DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac ConSep BatchSep

Check Status

15:17 06-04-2022

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Energy Analysis

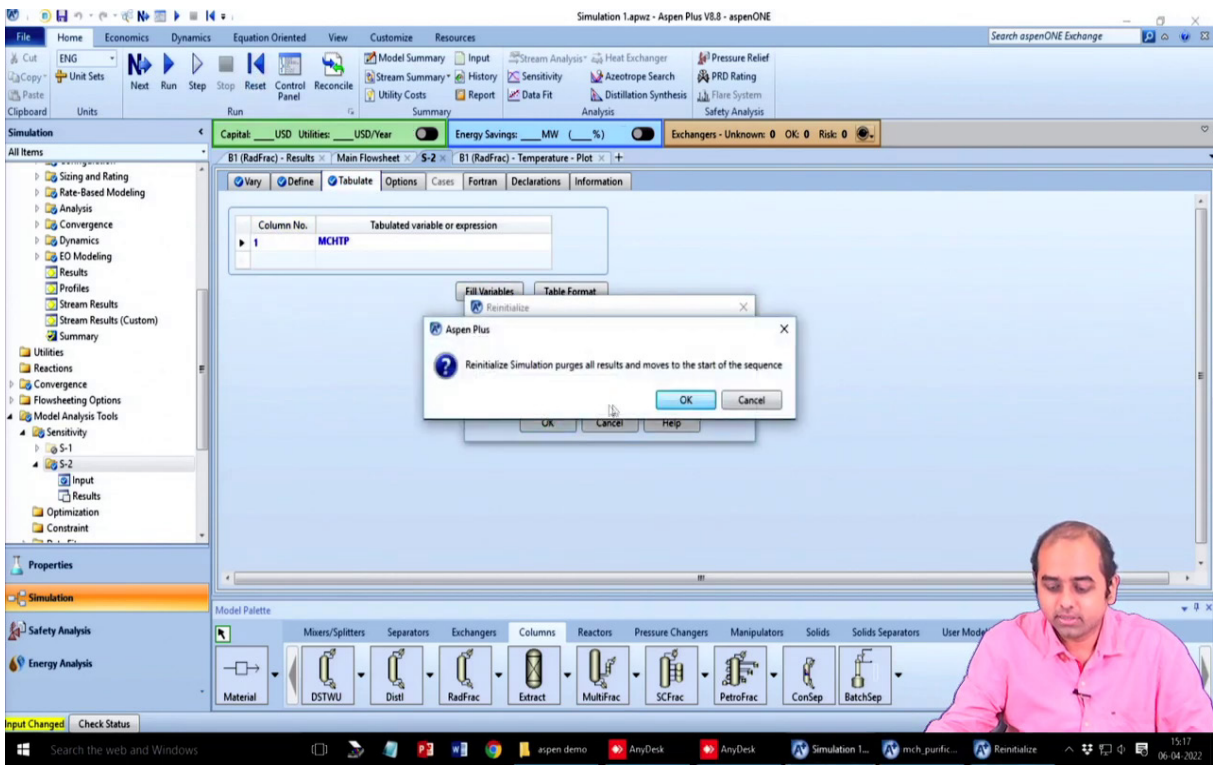
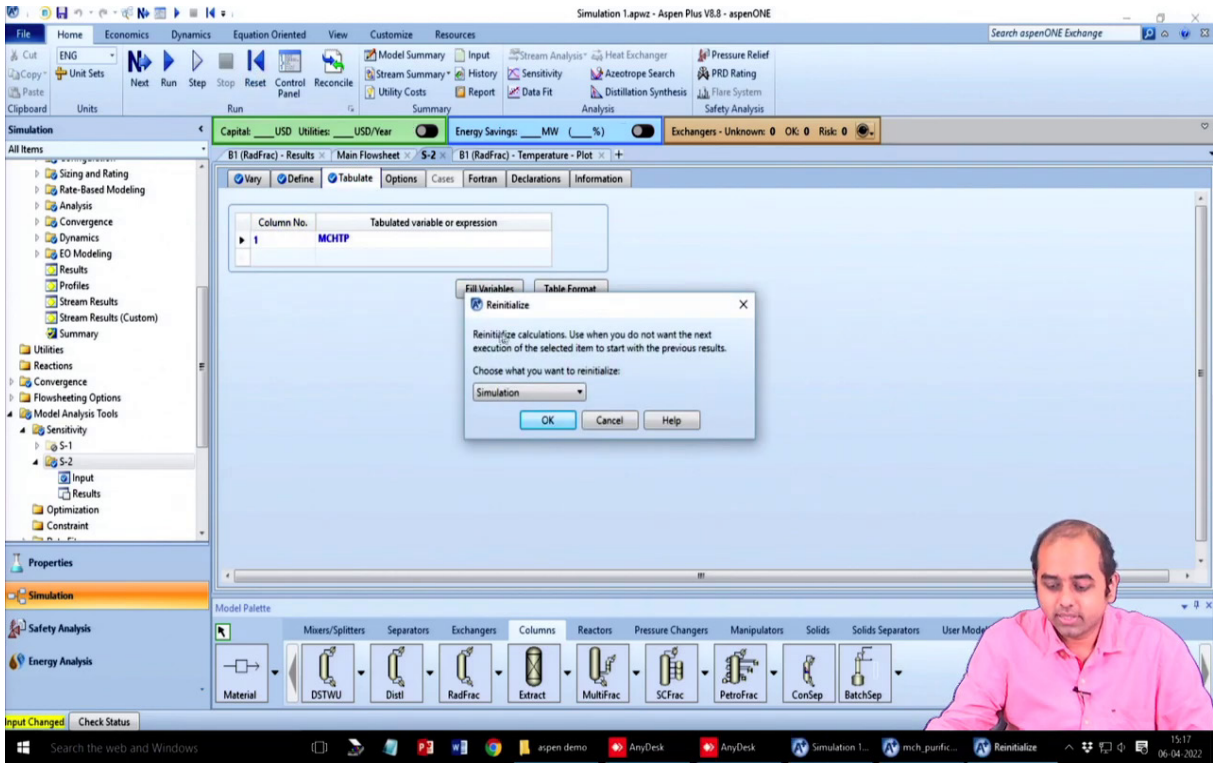
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Operating Costs
CO2 Emissions

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Energy Analysis

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Results Available Check Status

Search the web and Windows aspen demo AnyDesk AnyDesk Simulation 1.ap... mch.purificatio... 15:18 06-04-2022

Simulation 1.apwz - Aspen Plus V8.8 - aspenONE

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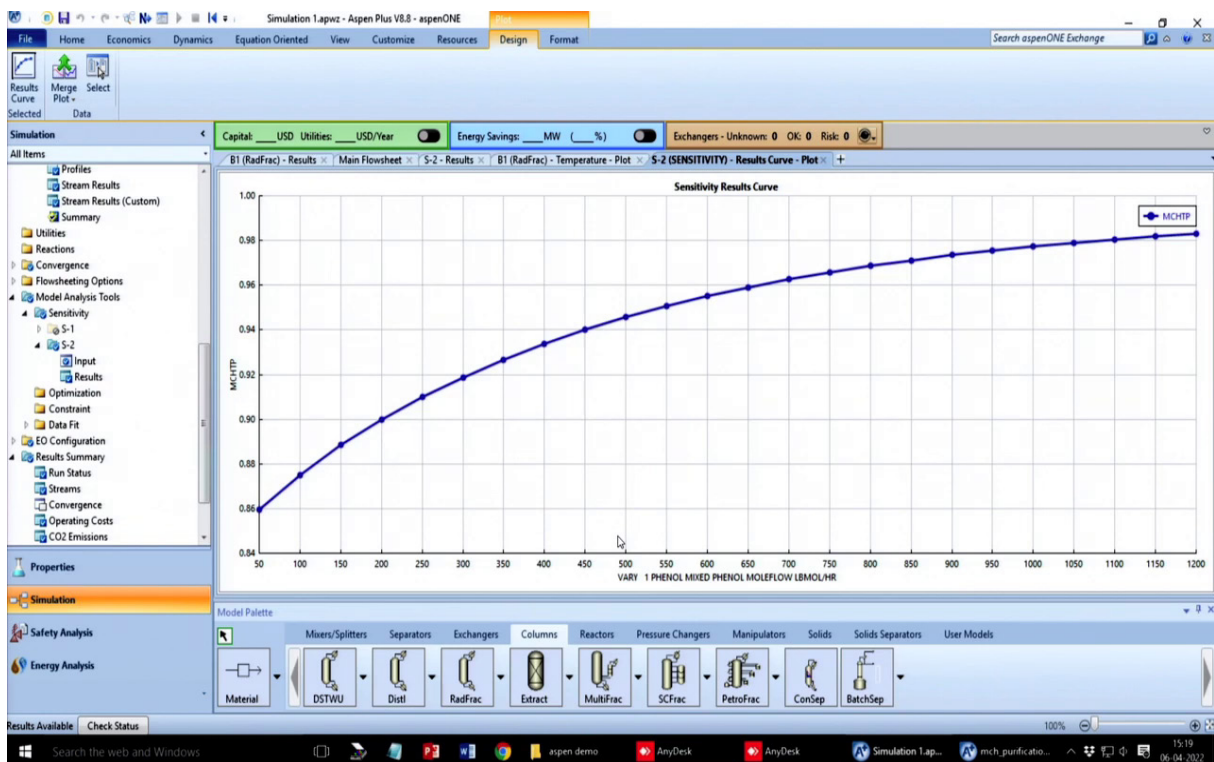
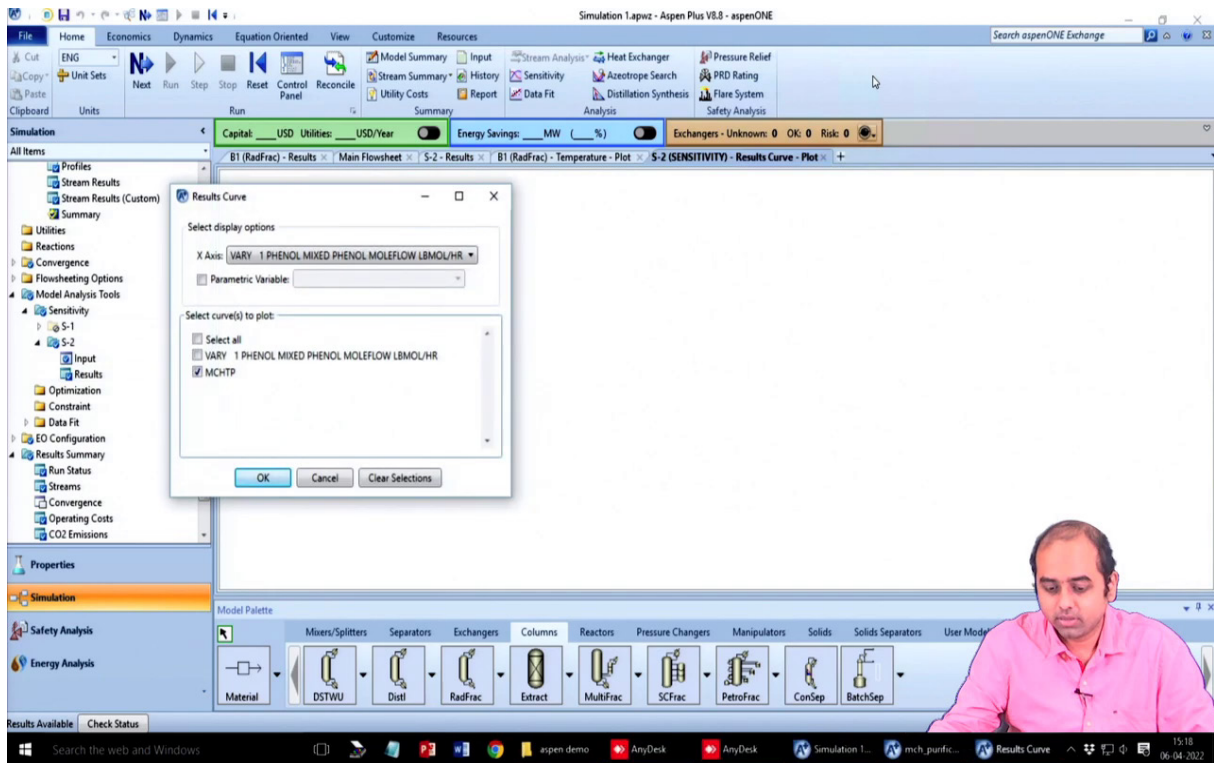
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Results Available Check Status

Search the web and Windows aspen demo AnyDesk AnyDesk Simulation 1.ap... mch.purificatio... 15:18 06-04-2022

Summary Define Variable Status

Row/Case	Status	VARY 1 PHENOL MIXED PHENOL MOLE LEB/MOL/HR	MCHTP
1	OK	50	0.859667
2	OK	100	0.875199
3	OK	150	0.888495
4	OK	200	0.899947
5	OK	250	0.909988
6	OK	300	0.918864
7	OK	350	0.926751
8	OK	400	0.933903
9	OK	450	0.940127
10	OK	500	0.945681
11	OK	550	0.950644
12	OK	600	0.955081
13	OK	650	0.959051
14	OK	700	0.962603



So, we will define another sensitivity. So, I will define a new one S2, and here I will try to define the phenol flow rate. Type as the mole flow, stream component so lower limit, let us say from 100 to 1200, let us say increment of 50 can start with 50. So, this ensures that the maximum value in the base case is by 1200. So, I start with 50 and goes up to 1200 and then

define the output variable that I want to track that is MCH top. And this is a stream. So, type mole fraction stream is MCH top component is methylcyclohexane.

Just fill variables. That is it. So, now reset the simulation and let us run it. So, once it is run, it shows the results are available. And now if you check the results of the sensitivity and just go with the plot, you will see that even with 50 phenol flow rate, which is like almost 25 percent or not 25 percent is in fact less than 15 percent of the total flow rate, total flow rate is 400. So, even with 50, so which is around 25 percent you will see that still the improvement is there.

And generally, the improvement, the fraction is increasing as you increase the 1200, but you can understand little is going to have a plateau after a certain value of the phenol flow rate. So, if you set your desired enrichment level is up to 0.95, then you can easily select from this curve that 450 would be sufficient or 500 would be sufficient to achieve 95 percent of the purity, thermodynamic limit is almost around 80 percent or 83 or 84 percent maximum.

So, I hope all of you get this basic understanding of a simple distillation column and how the sensitivity can be a very useful and a powerful way to calculate the optimum. You similarly can also carry vary the feed stage location that variable you can do can do the number of stage. You can also vary the reflux ratio in the sensitivity analysis. And can work out that essentially how the output variable or essentially the distillate mole fraction of methylcyclohexane is altered with varying the manipulated variable.

So, I hope all of you liked this demonstration. So, in the next class, we will talk about some other systems, particularly two systems coupled together, flash as well as reactors. Thank you. I hope all of you liked and enjoyed this.