

**Mathematical Modelling and Simulation of Chemical Engineering Process**  
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**Lecture 45**  
**Solving multiple units using Aspen Plus**

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**CONCEPTS COVERED**

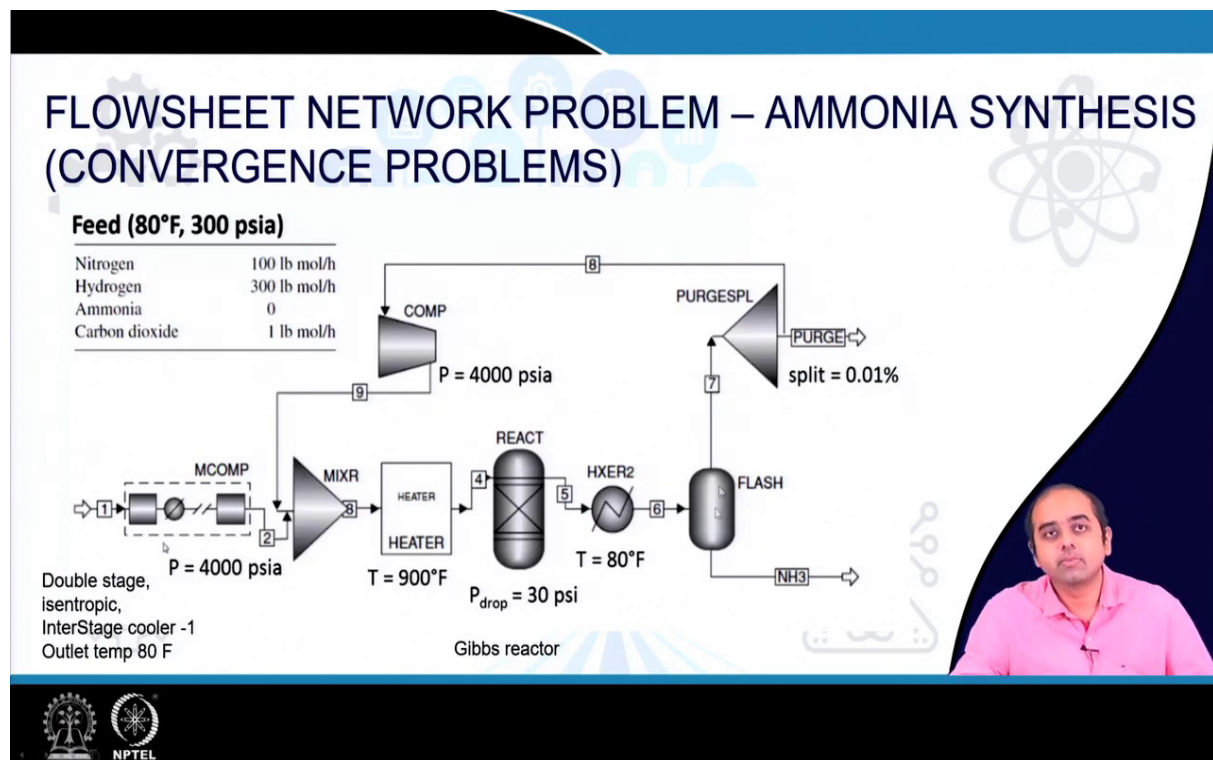
- ❖ **Multiple coupled units with recycle streams**
- ❖ **Solving complex network units and convergence issues**

The slide features a dark blue header with the title 'CONCEPTS COVERED' in orange. Below the header, two bullet points are listed. In the bottom right corner, there is a small video inset showing Professor Sourav Mondal. At the bottom left, there are logos for IIT Kharagpur and NPTEL.

Hello everyone. In this class we are going to talk about a complex network problem involving you know multiple units not two or three but multiple units and different types of units. So, this is regarding the process of you know ammonia synthesis or this classically known as the Habers-Bosch process. So, here the different units are actually coupled.

So, input of one stream goes to the output of one stream and then you also have some you know splitting recycles and because there are a lot of you know streams involved in this process convergence of this complex problem is very very critical issue. So, we will talk about the different types of convergence methods or like try to look into the different you know solver methodologies and how these convergence issues can be tackled and what is the background of the different types of you know convergence options or the different types of solution methods that are present.

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So, now let us go to the flow sheet of the problem of ammonia synthesis and this you can see that the feed that is denoted here in this first goes through you know multi stage compression because the feed is at 300 psia but this has to be compressed to almost 4000 psia. So, that is something too much extreme to be handled by a single stage compressor that is why multi-stage compressor is used. Then it goes to a mixer because there is a recycling stream coming and this idea of recycling was originally proposed by Haber-Bosch. So, as to improve the conversion of the ammonia.

So, if you look into the ammonia synthesis you know the process, I am sure you must have studied this in your chemical technology class you will see that as far as the equilibrium is concerned you need to you know, you know if you apply high pressure the conversion will be more but there is one problem of the side reactions there is one problem of the side reactions that affects the ammonia formation a lot. Moreover, this ammonia production is an exothermic process but you need to operate this system at a high temperature.

So, as a result the single pass conversion is very low in this reaction to improve that single pass conversion what you do is that you increase your pressure, further for industrial you know feasibility the idea of recycling has been improvised. So, any unreacted components nitrogen particularly hydrogen is essentially recycled. So, as to improve the conversion or per pass conversion.

So, for the side reactions to be avoided side reactions normally goes to you know ammonia biurets and all those things which is to be avoided the temperature is increased. So, that the kinetics is faster and this byproduct formation is reduced but on the downside is that if you increase the temperature, is an exothermic reaction. So, the conversion is low to circumvent this problem you have this recycling as well as you know this high-pressure operation.

So, from the equilibrium knowledge or from the equilibrium you know idea or the concept this should not operate at high temperature but high temperature is used to faster the kinetics. So, that the byproduct formation can be reduced. Now, you see in this case because there is a recycling stream that is why the merger or the mixer you know component is used and this recycling stream is also pressurized at the same pressure.

So, either this is mixed. So, generally that is what it is done because the output of the system whatever we are getting is already you know quite well pressurized even though it is not up to 4000 psia but it is quite well pressurized. So, mixing that stream to the feed stream it will lead to a lot of loss of energy instead you can use a single stage compressor to just increase the pressure little bit and bring it up to 4000 psia and mixed with pressurized stream, feed stream in the mixer then it is passed through a heater then through a reactor.

So, this feed whatever is present is let us say a very low temperature that has to be heated up to almost 900 degree centigrade that is close to the reactor temperature and next we have the you know this heater is essentially HXER2 is essentially the cooler. So, bring it down to the temperature lower temperature. So, that you can operate the flash.

So, flash is a easy way of separating the you know ammonia with the other gaseous components nitrogen hydrogen with easily in the flash or this you know in the flash it will just get you know vaporized and it will just move out now in this top there is a need for a split or a splitter.

So, why the splitter is necessary is because you do not wish to recycle entire unreacted compounds why? because normally the source of hydrogen in any ammonia synthesis the source of hydrogen is from the refinery from the reforming or the water gas shift reaction. So, there is a possibility of some hydrocarbon-based compounds which is already present in the hydrogen and that you know separation or to get a very high purity hydrogen is not economically feasible.

So, if you do not have these splits then this hydrocarbon waste particularly carbon dioxide other hydrocarbons will essentially get accumulated in the system for that split is necessary. Split will also help you to balance the stoichiometric amount of course you are losing some amount of hydrogen see nitrogen is not costly but hydrogen is so you are of course losing some amount of hydrogen but please note that in this recycle stream on the top of the flash whatever you are getting that is the unreacted amount is not in the same stoichiometric ratio.

So, whatever you are putting it into the feed you may be inserting in the stoichiometric ratio that is why that feed composition you see that nitrogen when nitrogen is to hydrogen is one is to three but in the recycling stream that whatever this you are getting in the from the recycling stream may not be in the same proportion.

So, this will affect the stoichiometry. So, it is better to you know have some split in the system or some purging is in this system even though we are losing some amount of hydrogen from the system but still it is desirable so that the you know this part the recycling stream is not excessive to the system.

That is the reason why we do have this split or this purge part here and this just point zero one part of the fraction most of them is actually reutilized. So, hydrogen is something that you cannot actually throw it out. So, even though there are impurities in the form of hydrocarbons but it is not a good idea for the economic feasibility to just you know purge out the entire hydrogen that is not a good idea that is why the recycling is needed also recycling is helpful to improve the you know per pass conversion efficiency that is why this becomes industrially a viable process.

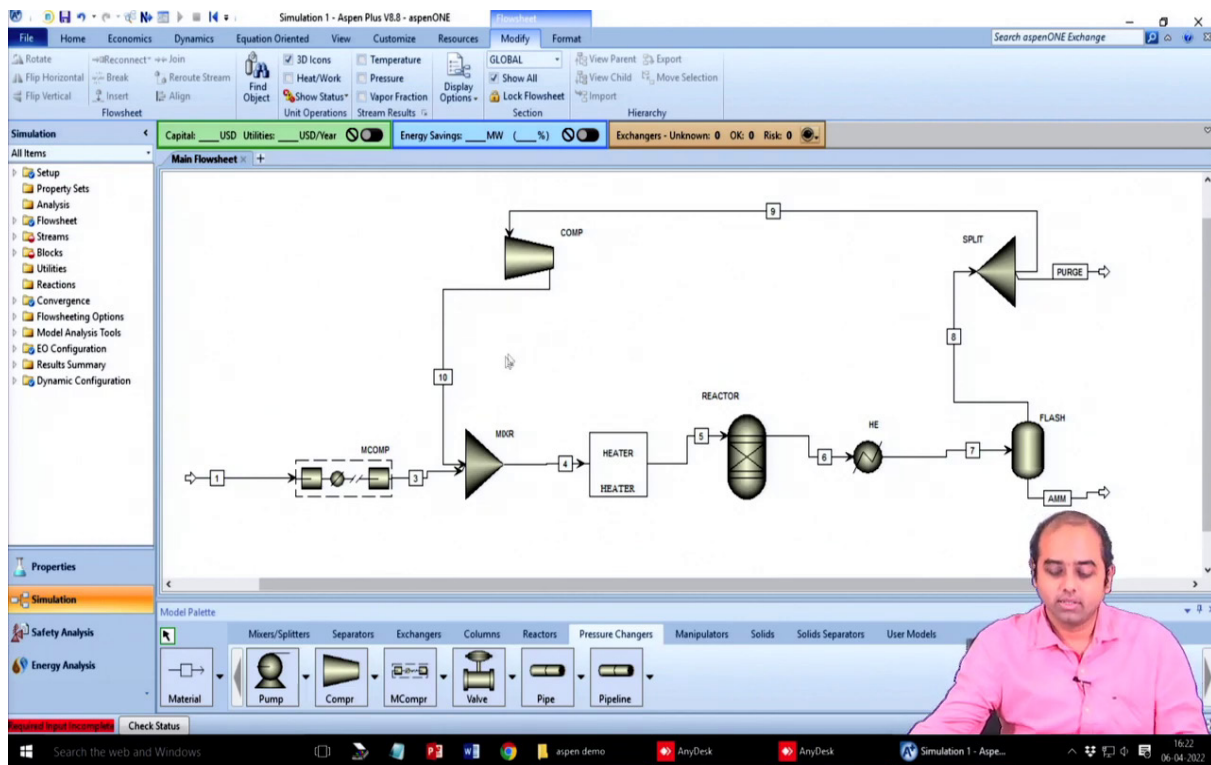
So, please note down all the you know process conditions it is a double stage compressor and the compressor and heaters are one of the expensive parts of the as well as the reactor also but apart from the reactor it is the compressor and the heaters not heaters I would say by attention the compressor which is the most expensive equipment in this system or the most energy consuming system heater is also true but compressor is one of the very high consuming particular double stage compressors are very high energy units it also needs some inter stage cooler one inter stage cooler and outlet temperature of the cooler should be around 80 degree Fahrenheit, reactor drop is 30 psia, temperature of the heater is 900 and then the cooler is 80 in terms of Fahrenheit and the feed conditions are mentioned.

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The screenshot shows the Aspen Plus V8.8 - aspenONE software interface. The main window is titled "Components - Specifications" and displays a table of selected components. The table has four columns: Component ID, Type, Component name, and Alias. The components listed are N2, H2, NH3, and CO2, all of which are of the "Conventional" type. Below the table are buttons for "Find", "Elec Wizard", "User Defined", "Reorder", and "Review". The left sidebar shows a tree view of the software's structure, including "Setup", "Components", "Methods", "Estimation", "Analysis", "Customize", and "Results". The bottom status bar indicates "Required Input Incomplete" and "Check Status".

Component ID	Type	Component name	Alias
N2	Conventional	NITROGEN	N2
H2	Conventional	HYDROGEN	H2
NH3	Conventional	AMMONIA	NH3
CO2	Conventional	CARBON-DIOXIDE	CO2

The screenshot shows the Aspen Plus V8.8 - aspenONE software interface with the "Methods" window open. The window is divided into several sections: "Property methods & options", "Method name", and "Modify". The "Property methods & options" section includes fields for "Method filter" (COMMON), "Base method" (UNIQUAC), "Henry components", "Petroleum calculation options", "Free-water method" (STEAM-TA), "Water solubility" (3), and "Electrolyte calculation options" (with "Use true components" checked). The "Method name" section shows "UNIQUAC" selected. The "Modify" section includes options for "Vapor EOS" (ESRK), "Data set" (1), "Liquid gamma" (GMUFAC), "Data set" (1), "Liquid molar enthalpy" (HLMX103), "Liquid molar volume" (VLMX01), "Heat of mixing" (checked), "Poynting correction" (checked), and "Use liquid reference state enthalpy" (unchecked). The bottom status bar indicates "Required Properties Input Complete" and "Check Status".



Now first let us try to prepare this sheet flow sheet and then try to see that I mean what happens when you try to solve it let us first work it out frame this flow sheet in the aspen platform. So, let us choose a blank simulation, first let us try to place the different units then connect the streams. First thing is to do is to have the specification of the streams or the chemicals that are involved I can write N2 and it will take nitrogen good H2 will take as hydrogen NH3 I can write is the ammonia and CO2 is the carbon dioxide methods base method let us choose UNIFAC that is done all specifications are set.

Next let us go to the simulation tab try to place the different units here the first one is the multi-stage compressor. So, m compressor multi-stage compressor that is the compressor block then we have one mixer. So, I am placing the components first then I am trying to you know put I have the, these connections, heater block, shifted little bit on the side after the heater we have the reactor note that this is a Gibbs reactor here because there could be several types of reactions by products etcetera could be possible it is not possible to explicitly specify one particular reaction in this case.

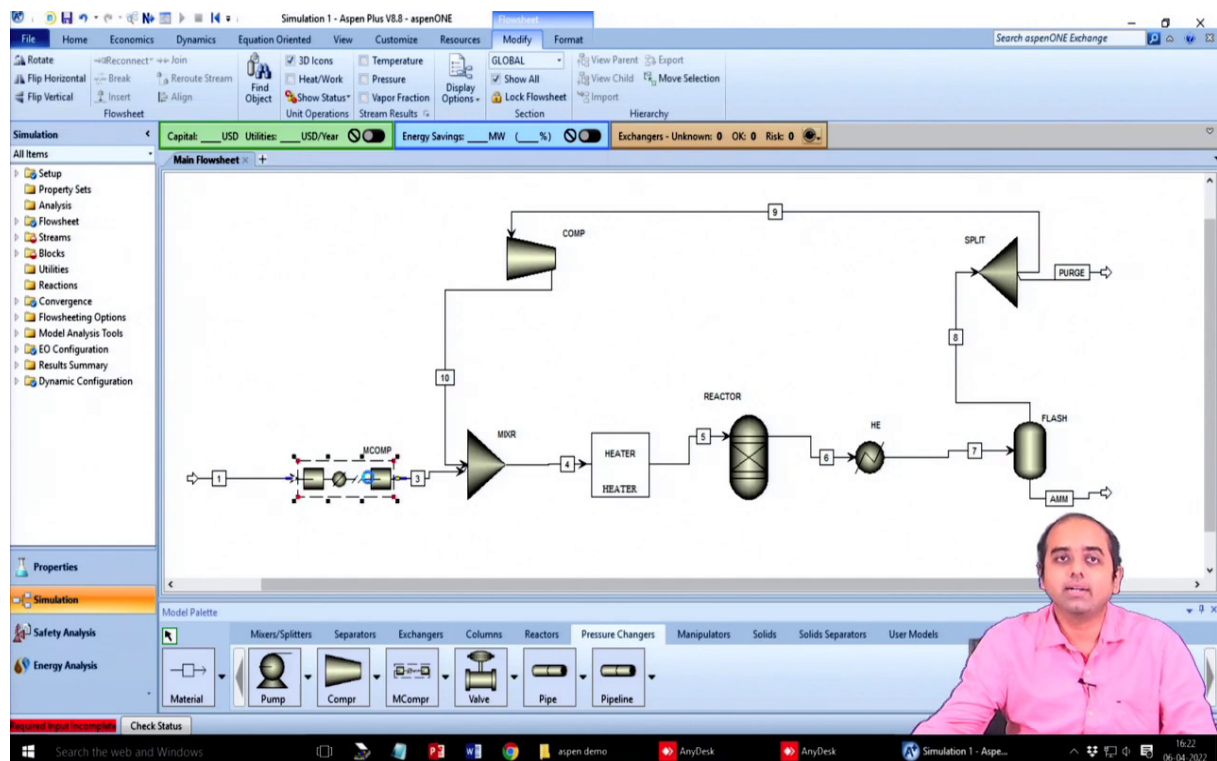
Then we have the cooler essentially this is the cooler, then the flash, on top of the flash we have the again splitter and we have one more compressor, let us rename the different blocks that would be helpful to identify later on and for ourselves this is mixer, this is heater, this is the reactor, this is let us say the heat exchanger, this is a flash and this is the splitter and this is the compressor. Now, it is time to connect the streams.

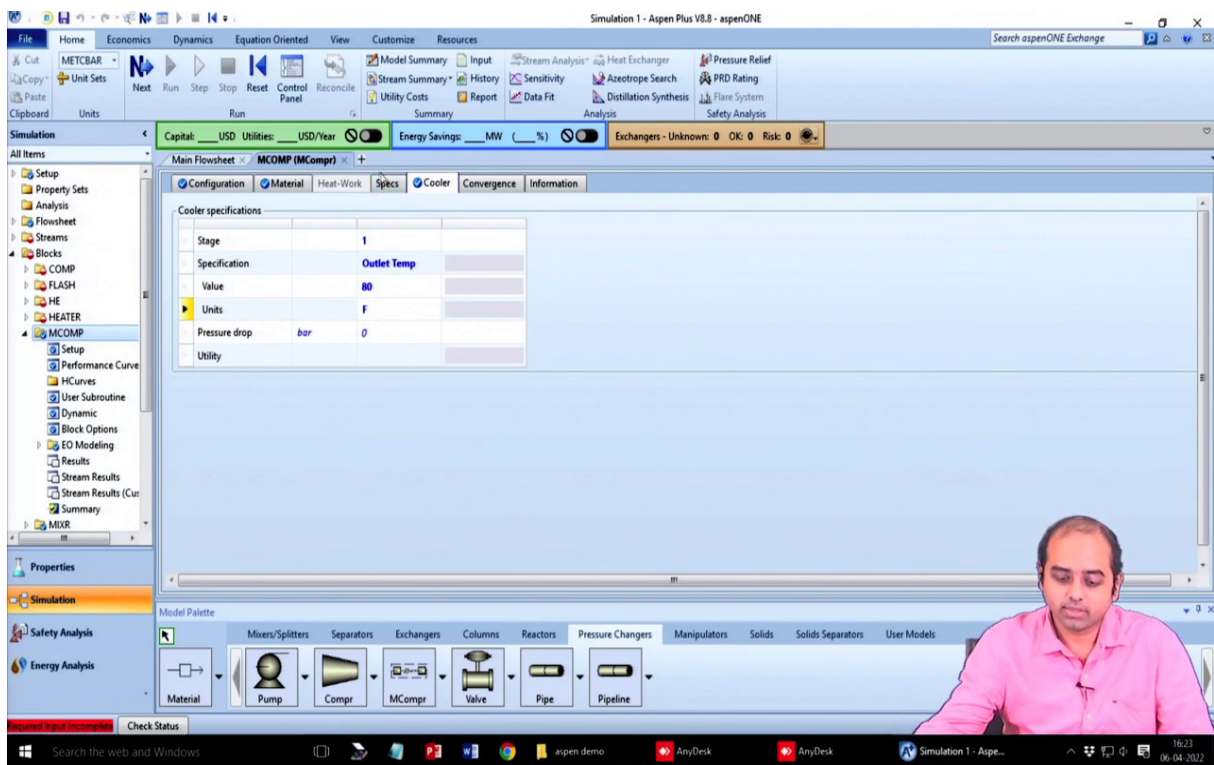
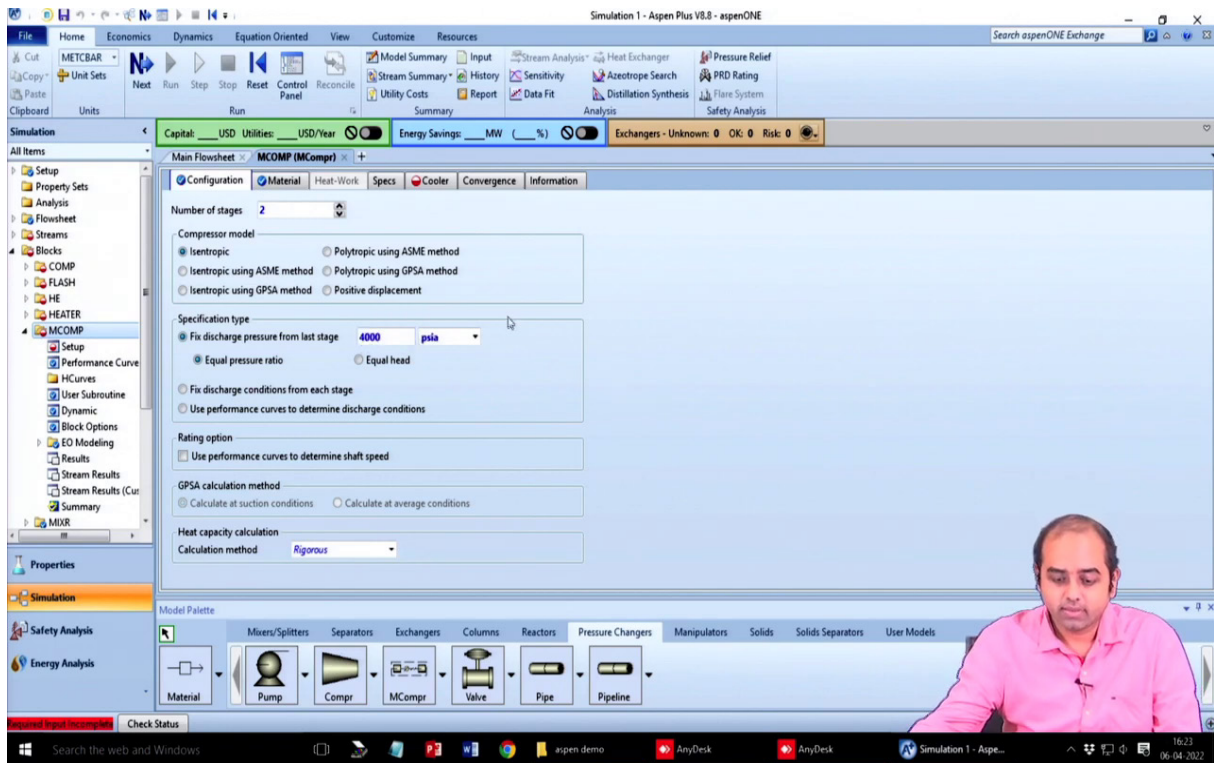
So, this is our feed to the compressor, then output of the compressor goes to the mixer of course there will be one recycling stream. So, you see now here still the red arrow is showing. So, that means this stream is not connected properly. So, let us delete it and connect it again. Now, it is connected properly next is from here to the heater, then from the heater to the reactor, Gibbs reactor, from the reactor to the heat exchanger, from the heat exchanger to the flash, then from the flash to the splitter and from the splitter we have it here.

So, if you just you know click and click the next one it will automatically you know show you the best possible arrows you need not to worry about how the arrow is placed so, nicely and then from the output of the compressor. So, make sure that the compressor input and the output is connected properly. So, this is the compressor it can also worked as the depressurizing unit also the other way around output goes to the mixer.

So, two this is the big recycling stream actually. So, this is the purge stream, let us write that as P U R G E purge that is the purge stream and this is the feed stream let us keep it as one. So, it is all sequentially numbered now it is time to specify the and so bottom of the flash is not done. So, at the bottom you will getting ammonia, that is the main component.

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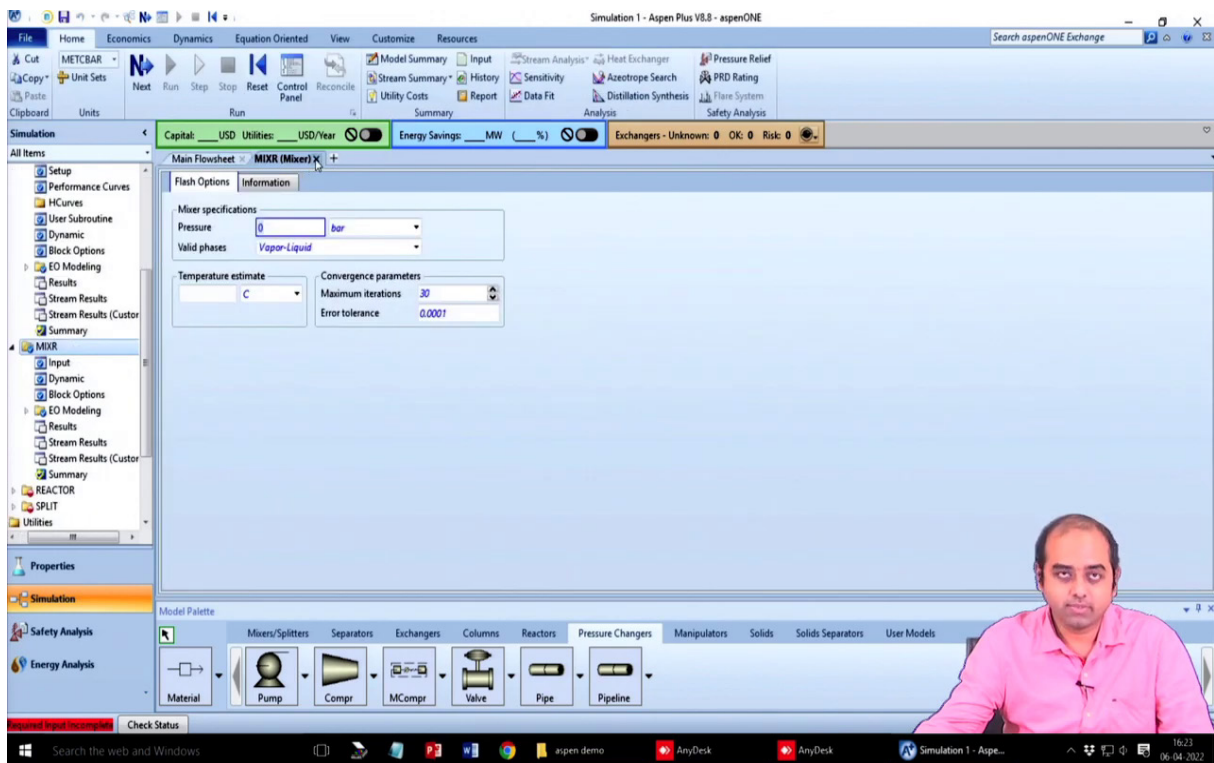
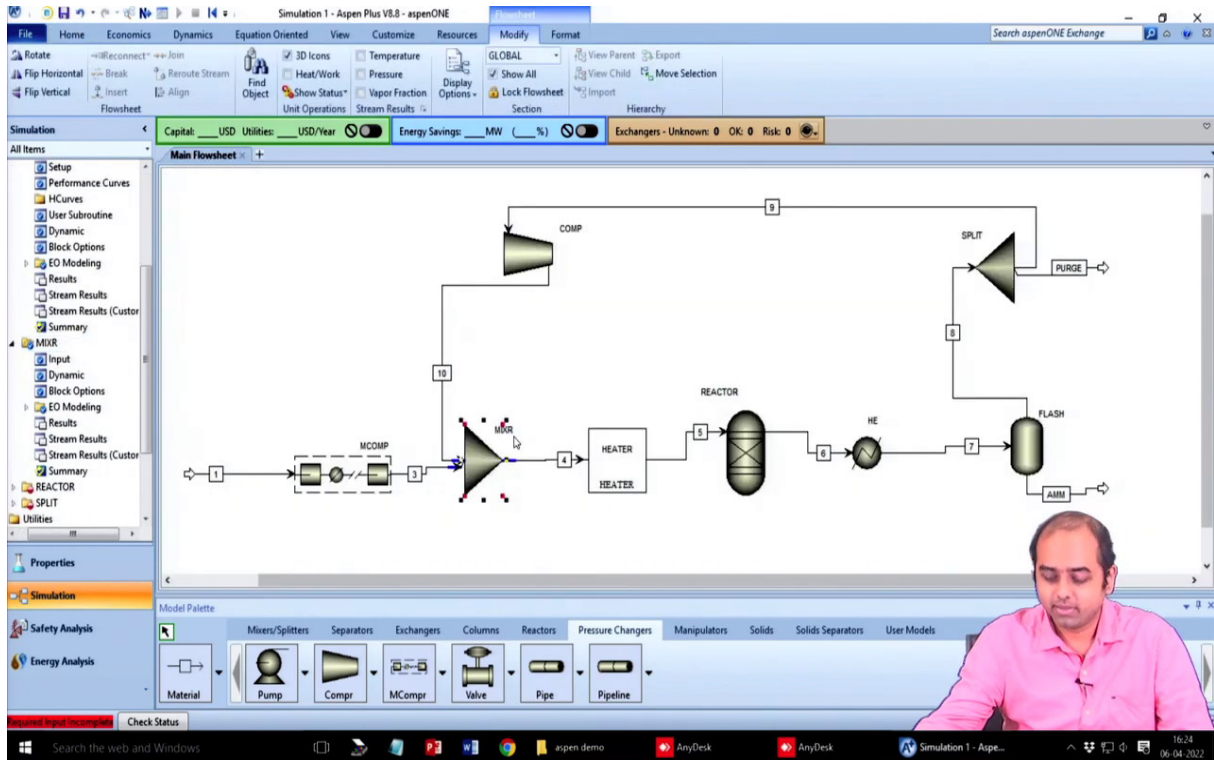


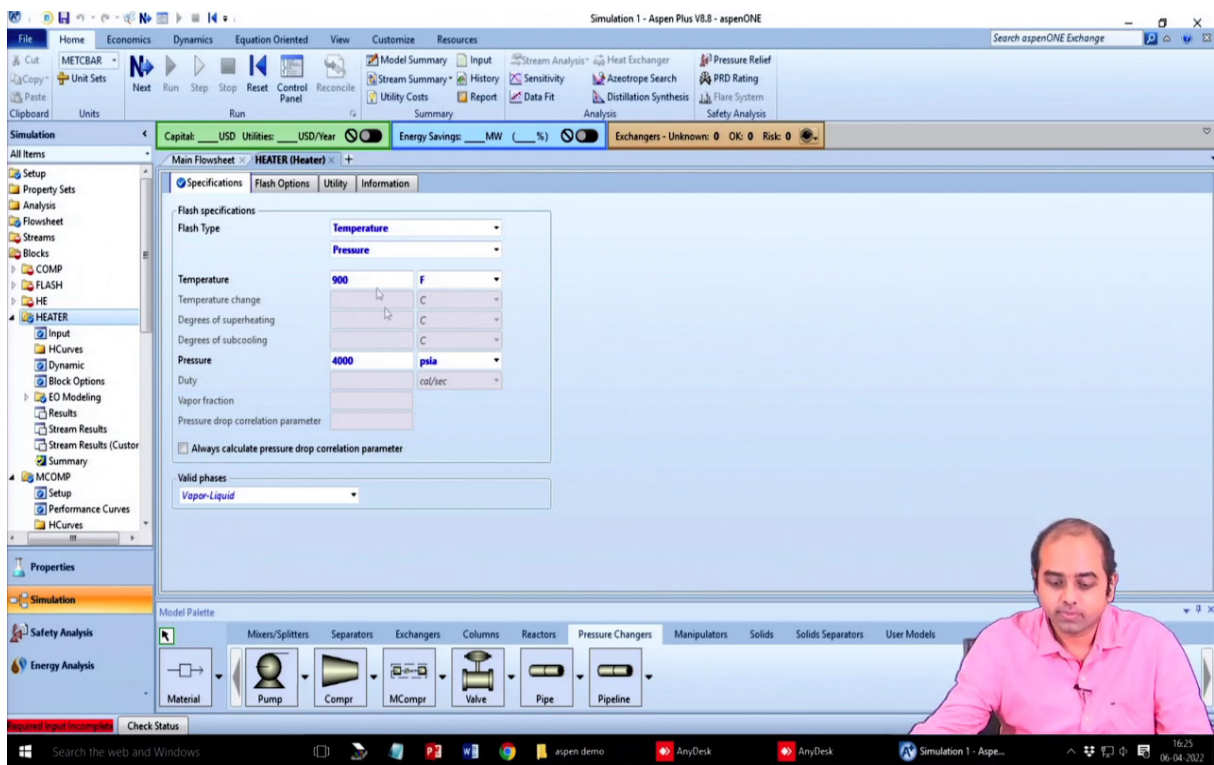
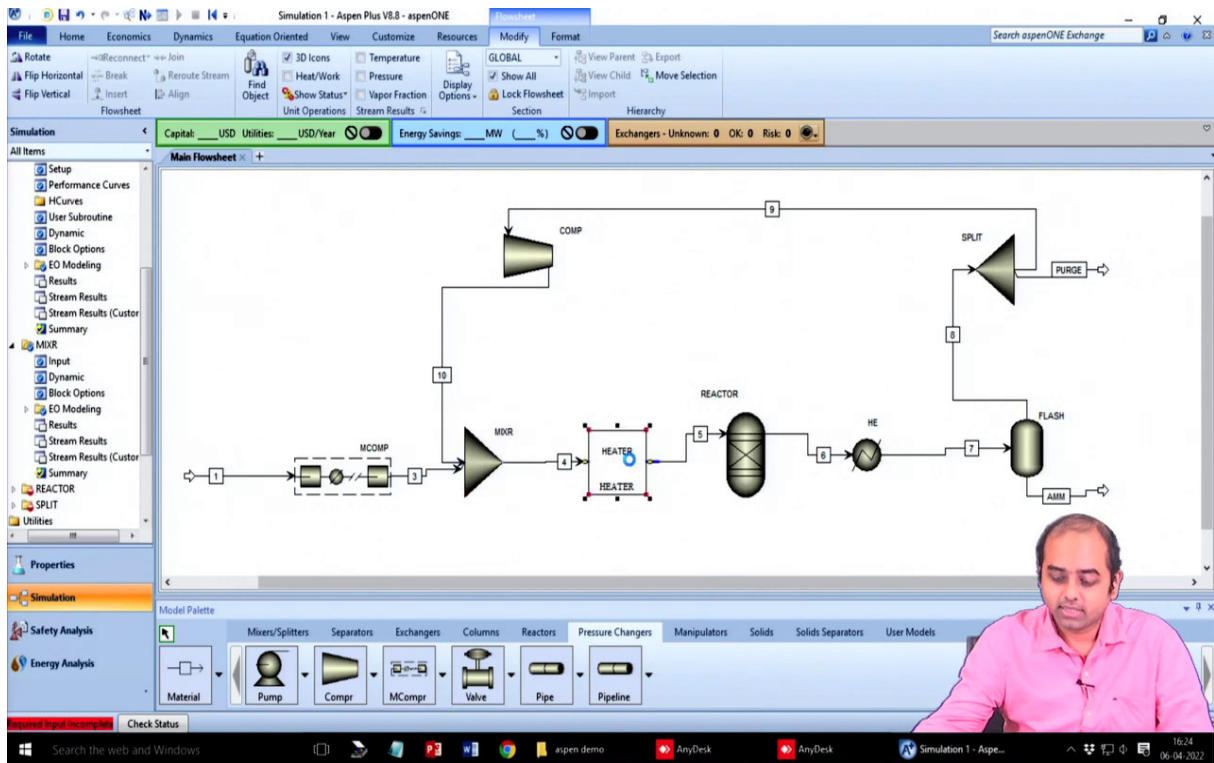
Now let us try to specify or the different you know the properties of the individual blocks as far as the problem statement is concerned. So, first is the multi-stage compressor. So, if you see in the multi stage compressor, the number of stages is double stage. So, two, next is isentropic and we have the fixed discharge from the last stage let us specify as psia, next is the cooler. So, cooler is one specification outlet temperature value 80-degree Fahrenheit. So,



often cooling is very important for you know multi stage compression multi stage compressor is specified.

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Next mixer or mixer there is no condition that needs to be specified which is only merger of the streams. Next is the heater. So, for the heater the temperature needs to be specified as 900 Fahrenheit. Pressure is so if you do not specify any pressure then it suggests that there is no pressure drop in the system. So, if you note this here. So, it is if the outlet pressure it says that the you know if you specify any pressure and then it becomes like the pressure drop.

So, we do not specify any pressure I hope this is correct no it still needs to be specified 4000 psia, is the same pressure we have fixed as so there is no pressure drop. So, if you specify something in minus it will act as a pressure drop but if you specify in terms of you know positive units it is the absolute pressure that it will choose.

(Refer Slide Time: 18:40)

The screenshot displays the Aspen Plus V8.8 simulation environment. The main window shows a process flow diagram with several units: a compressor (COMP), a mixer (MIX), a heater, a reactor, another heater, a split stream, a flash drum, and a purge stream. The simulation status bar at the bottom indicates 'Required Input Incomplete' and 'Check Status'. The taskbar at the very bottom shows the system clock as 16:25 on 06-04-2022.

The screenshot shows the 'REACTOR (RGibbs)' properties window in Aspen Plus V8.8. The window is set to 'Specifications' and displays the following information:

- Calculation option:** Calculate phase equilibrium and chemical equilibrium
- Operating conditions:**
  - Pressure: -30 psia
  - Temperature: 900 F
  - Heat Duty: col/sec
- Phases:**
  - Maximum number of fluid phases: [dropdown]
  - Maximum number of solid solution phases: [dropdown]
  - Include vapor phase
  - Merge all CISOLID species into the first CISOLID substream

The taskbar at the bottom shows the system clock as 16:26 on 06-04-2022.



Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

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

Main Flowsheet: HE (Heater)

Flash specifications

Flash Type: Temperature Pressure

Temperature: 80 F

Temperature change: C

Degrees of superheating: C

Degrees of subcooling: C

Pressure: 0 psia

Duty: cal/sec

Vapor fraction:

Pressure drop correlation parameter:

Always calculate pressure drop correlation parameter

Valid phases: Vapor-Liquid

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

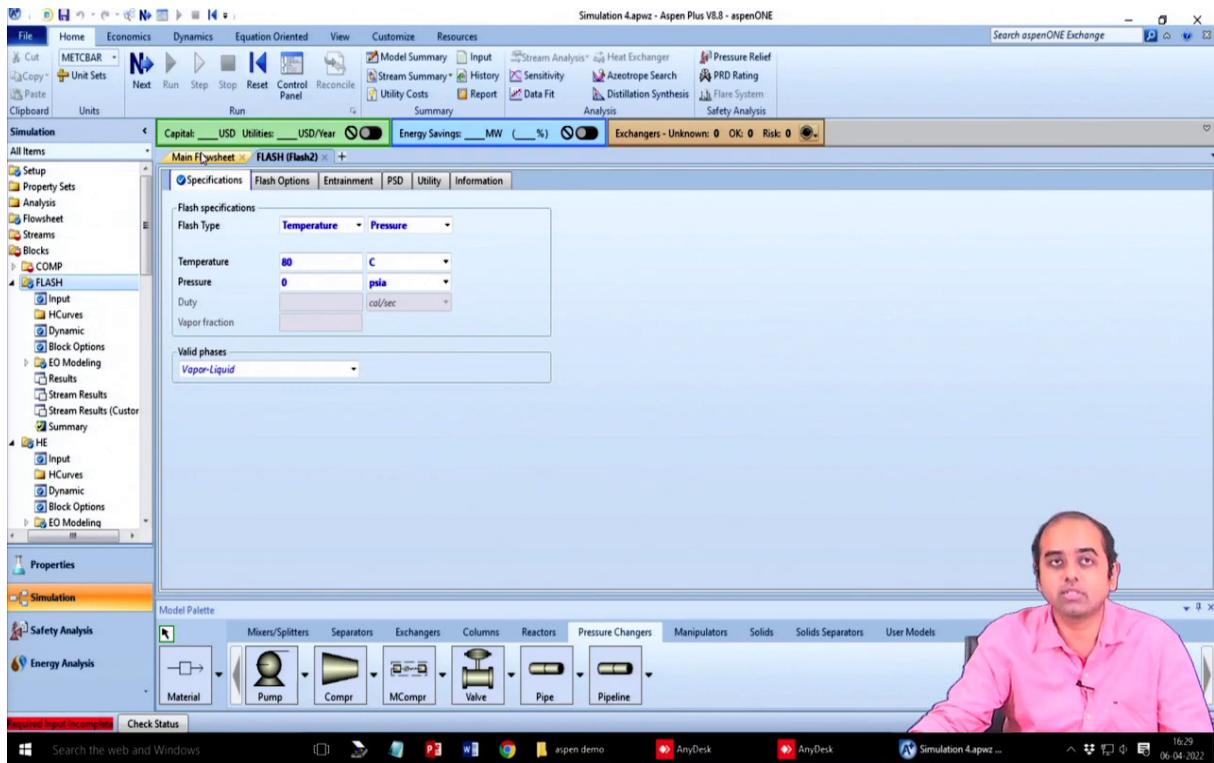
Simulation 1 - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

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



Then is the heat exchanger again in the heat exchanger we specify the temperature 80-degree Fahrenheit and this is or I can write the value as 0 that means there is no pressure drop in this part. Similarly, I can just rephrase this heater to 0. So that, there is no pressure drop we consider. Any other value will choose as the absolute units and negative means pressure drop let us go to the flash, flash, the temperature of the flash is.

So, the flash temperature is 80 degree that is the output of the heat exchanger and pressure is the same as it is from the heater or from the reactor whatever we are getting we do not change any of the pressure just reduce the temperature and in the case of the heater instead of specifying temperature you can also specify the heat duty in terms of 0 as 0 btu per hour.

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Simulation 4.apwz - Aspen Plus V8.8 - aspenONE

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

Main Flowsheet: FLASH (Flash2)

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

Simulation 4.apwz - Aspen Plus V8.8 - aspenONE

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

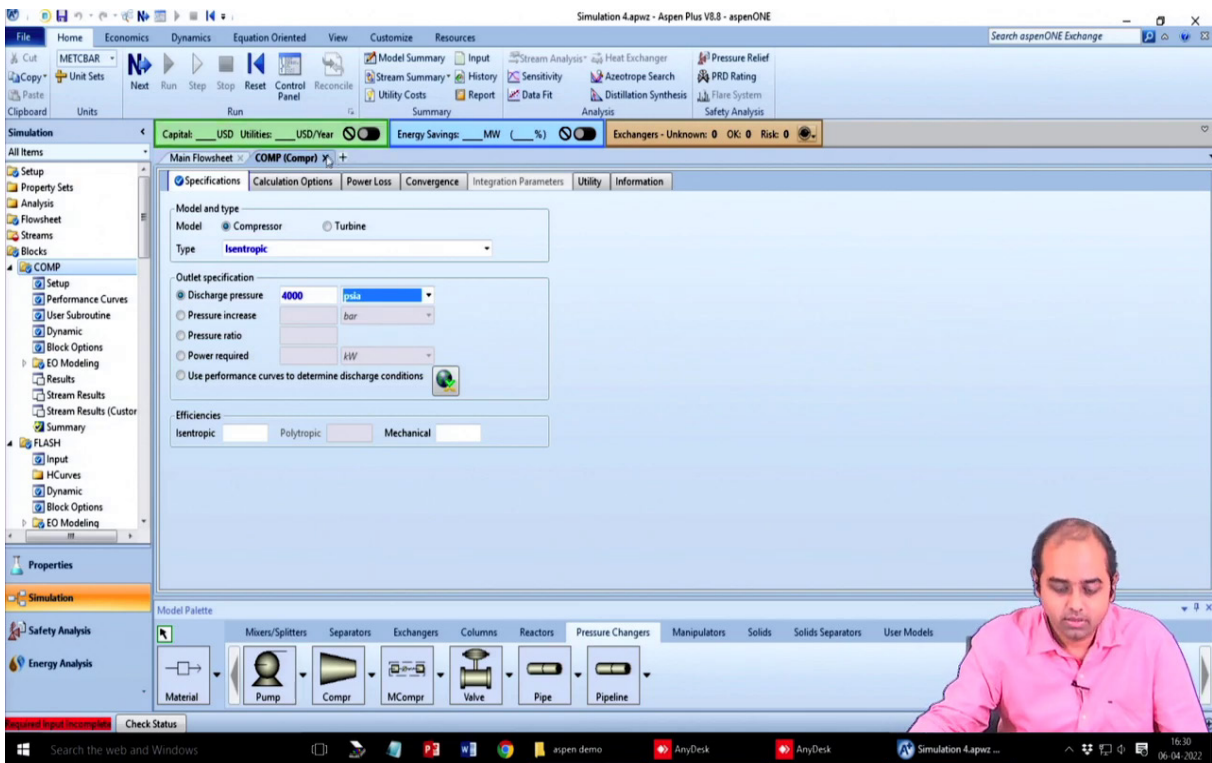
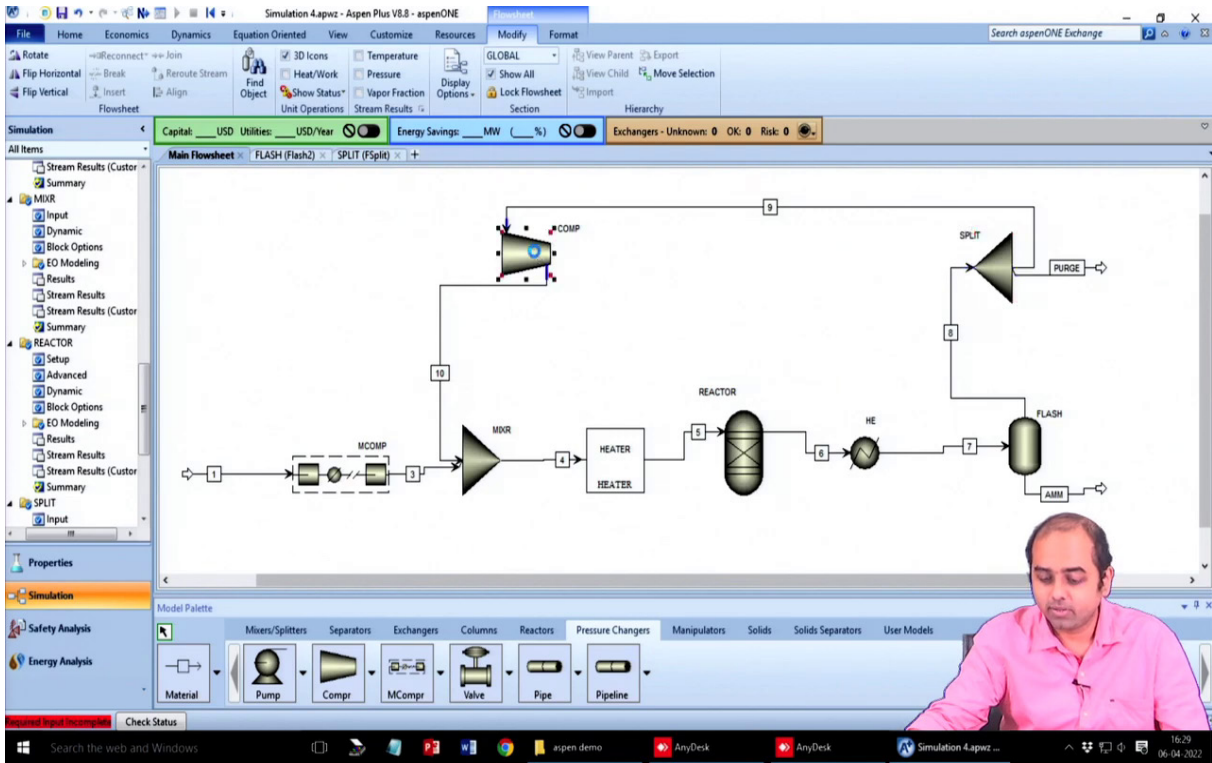
Main Flowsheet: FLASH (Flash2) | SPLIT (FSplit)

Specifications Flash Options Key Components Information

Flow split specification for outlet streams

Stream	Specification	Basis	Value	Units	Key Comp No	Stream order
9						
PURGE	Split fraction		0.0001			

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

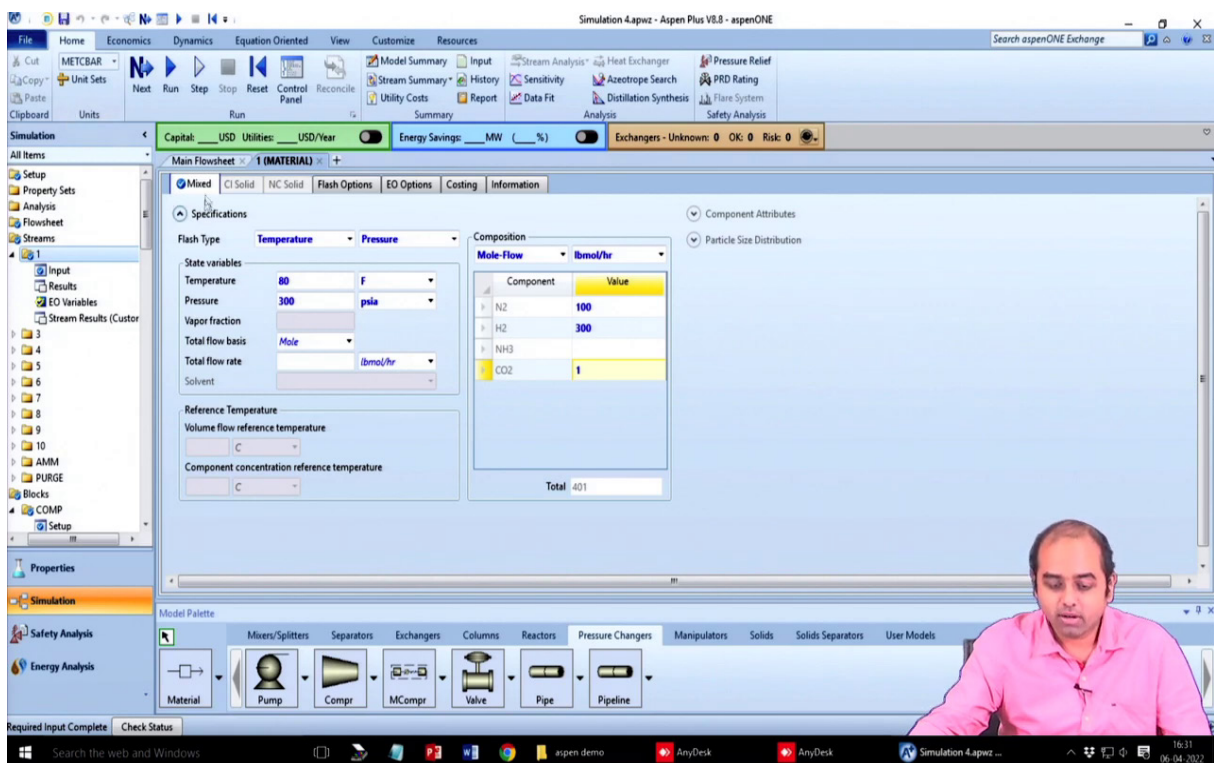
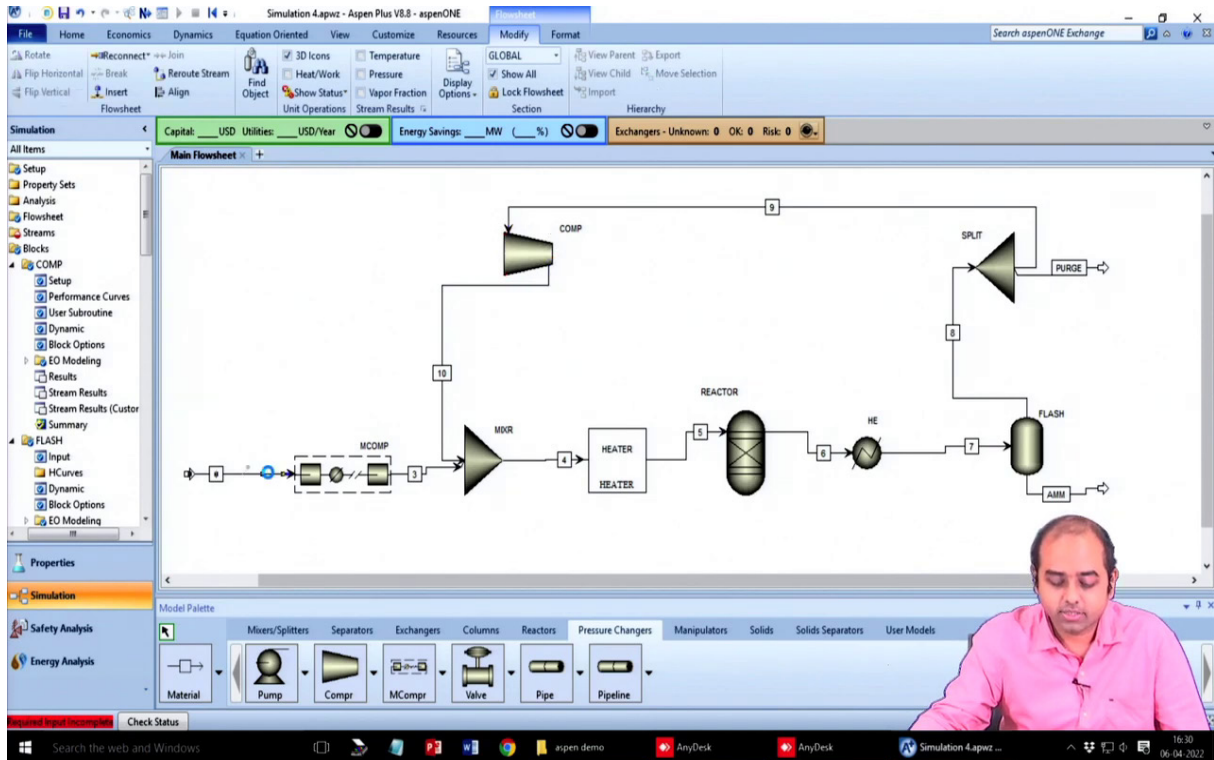


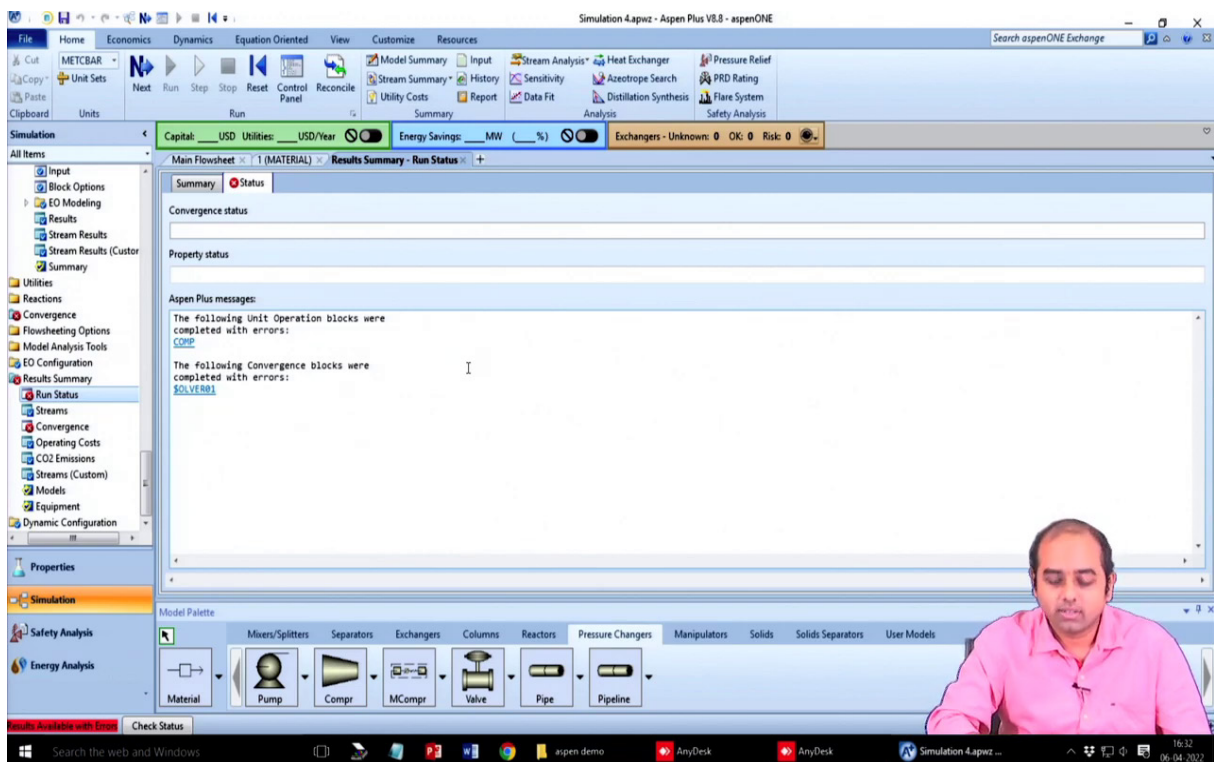
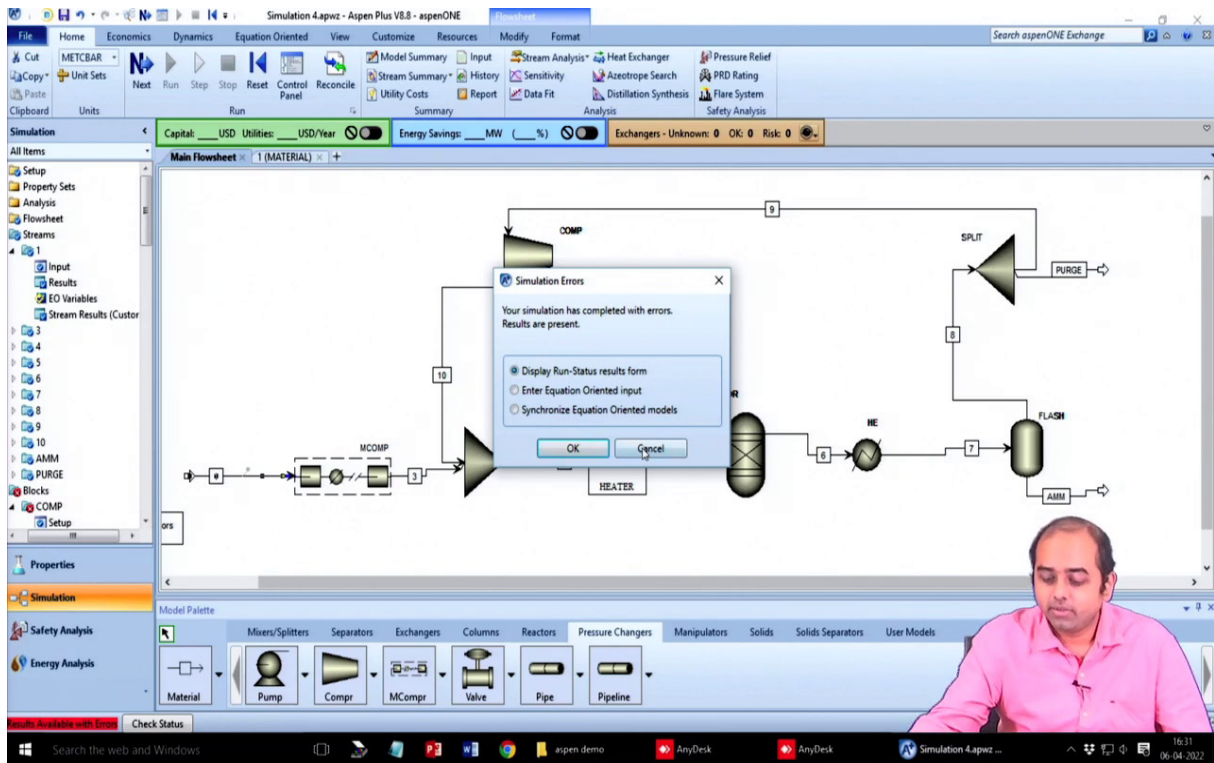
Next is the split. So, it will ask for the split fraction. So, the split fraction is this stream as the purge stream. So, that is 0.00, 01 that is 0.01 percent and then the compressor. So, isentropic compressor, discharge pressure we write 4000 psia just to compensate for you know any loss in the pressure during this process through the reactor I mean reactor there is a drop that itself we have specified after that it goes through flash, purging and all. So, this will compensate



the pressure but here the pressure change is not much that is why a single stage pressure compressor is more than sufficient here.

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Next, we have to specify the streams. So, the stream temperature is 80-degree Fahrenheit and pressure is 300. So, there is already it is pressurized before feeding to the compressor, psia and total flow rate we define in terms of English units the pound moles per hour and we say that either we can write the molar flows or molar flow rate as pound moles per hour. So, nitrogen is 100, hydrogen is 300 there is no ammonia carbon dioxide is one, 1 is 0.

So, this is the individual component molar flow rates that I have specified as the feed. So, now this required input is complete it is showing the status now let us try to run the simulation for this case and see what happens. So, let us run it. So, you see that it is showing that the simulation is completed with some errors and what is the error. So, it is showing that the error is associated with the solver block and as a result the you know this COMP is the compressor block.

(Refer Slide Time: 23:38)

The screenshot displays the Aspen Plus V8.8 interface. The main window shows the 'Run Status' tab with the following error message:

```

AFTER THE BLOCK HAD BEEN EXECUTED.

** ERROR
Convergence block SOLVER01 did not converge
normally in the final pass

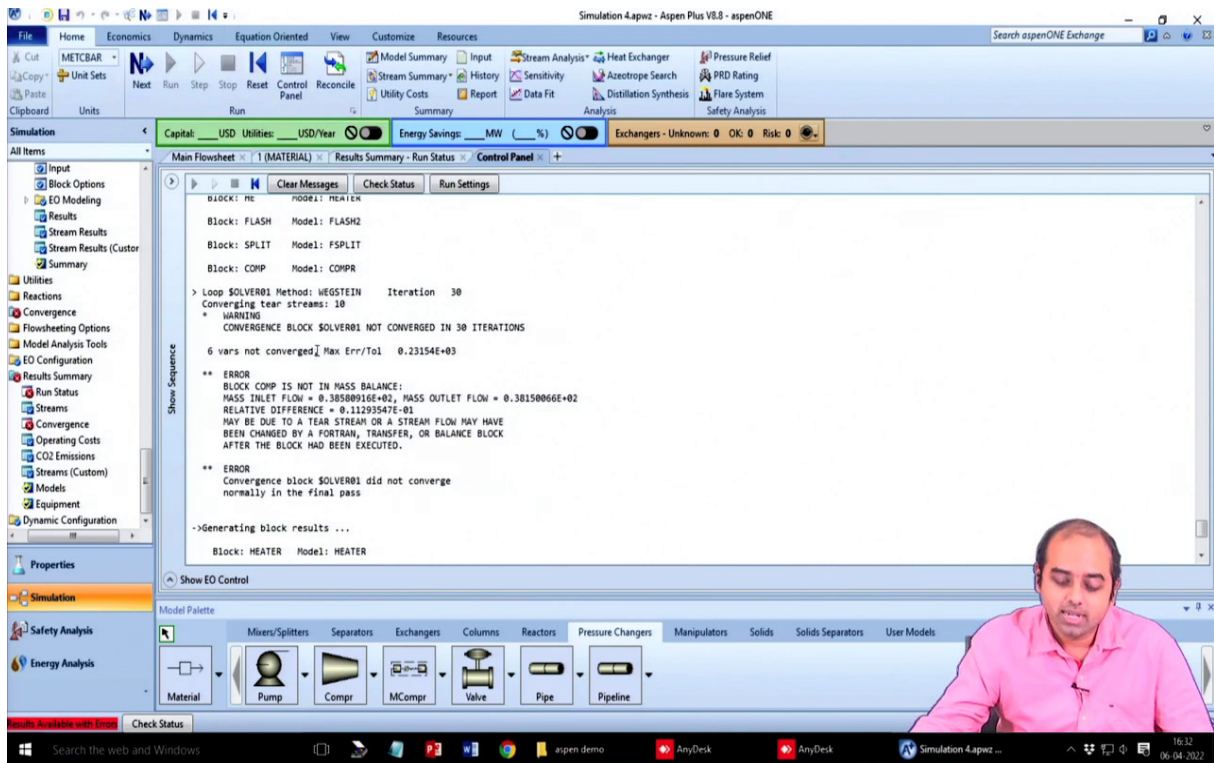
->Generating block results ...
Block: HEATER Model: HEATER
Block: HE Model: HEATER
->Simulation calculations completed ...

*** No Warnings were issued during Input Translation ***

*** Summary of Simulation Errors ***

Physical Property System Simulation
Terminal Errors 0 0 0
Severe Errors 0 0 0
Errors 0 0 2
Warnings 0 0 1
  
```

The 'Model Palette' at the bottom shows various unit operation icons, including 'Compr' (Compressor), which is the block associated with the error. The taskbar at the bottom indicates the system time as 18:32 on 06-04-2022.



So, compressor block fixed issue with the convergence you can also see the control panel and see the detailed you know results actually. So, almost after 30 iterations, still the you know the description that it is showing that the compressor block which is the compressor present in the recycling stream is not in mass balance. So, there is a violation of the mass balance condition and the relative difference is 0.01 which is above the tolerance maybe due to a tear stream or a stream may have been changed by the transfer during the recycling or whatever.

So, convergence there is the issue this convergence did not happen finally and that is why you know this this this simulation failed to be executed successfully. So, now let us look into the issue of what are the possible you know things with the convergence. So, what essentially the tier stream. So, let us try to you know learn about these shear streams the difference convergence methods in this case what are the different options.

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Convergence

Tear Stream: Recycle loop is the tear stream by default

Flowsheets with recycle loop specification are solved iteratively in Aspen Plus.

Convergence Block

Sequence.

So, let me just help you here. So, the thing that we encounter in convergence is about the Tear stream. A Tear stream could be any stream in the system but generally in this or in any process having recycling's recycle loop is the is considered as the tear stream by default. So, in this Tear stream. So, what essentially this Tear stream means for the solvers essentially in the tear stream you try to compute all the properties for example its component flow rate, total molar flow rate, mass flow rate etcetera pressure enthalpy are computed iteratively and based on these values the other streams are satisfied from the mass balance.

So, that is what we essentially mean by the tear stream. So, it can be any stream in the in the loop or in the system but generally the recycling stream is actually specified. So, any solution involving or any model involving recycling always solves by iterations, let me just write it down. Flow sheets with recycle loops specification are solved iteratively in Aspen Plus.

Next there is something known as the convergence block. So, it is essentially in the convergence block you have the different convergence options and the different convergence algorithms to be altered you know changing the tolerance etcetera. So, of course these things are by defined default but there is option to change them and it essentially determines I mean this convergence blocks essentially helps you to determine that how good is the gas or what is the level of the tolerance that you need or what are the different you know options or the methods that can be used if the default method fails and there is also something known as the

sequence. So, generally the sequence is from left to the calculation starts from the left to and it includes all the unit operations I mean all the unit operations are converged and then it proceeds to the next operation that is how the sequence happen.

(Refer Slide Time: 27:59)

**Convergence options.**

- \* Tear Convergence tolerance (default is 0.0001)
- \* Methods
- \* Parameter that affect sequencing
- \* Convergence parameter for each method

$$\left| \frac{X_{\text{assumed}} - X_{\text{calc}}}{X_{\text{assumed}}} \right| \leq \text{tolerance}$$

Trace Option is Cutoff. threshold is  $\text{tol}/100$

Now, what are the different convergence options? The convergence option that you have or that is something that can be modified one is the tear convergence tolerance. So, by default this is again relative default is 0.0001. Then you have the methods the different algorithms then you have the parameters that affect the sequencing and then you have the convergence parameter for each method.

So, this tear term convergence tolerance as I have said is relative. So, that means whatever is assumed for that value minus whatever that you have calculated in this iteration, divided by this assumed the absolute value should be less than the tolerance. There is also something known as the trace option by default this trace option something known as the cut off. So, the default trace option threshold is tolerance by 100.

So, what is this trace option. So, if the molar you know this mole fraction let us say if the mole fraction is less than the threshold. So, in this case if the tolerance is 10 to the power minus 4 if the mole fraction of a particular or the tear of the tear stream or particular

component is more than let us say sorry if it is less than this threshold that is tolerance by 100 in this case it is like 10 to the power minus 6.

So, that means some trace amounts is there. So, for those stress amount of chemicals or for the trace amount of the component we do not worry about its you know convergence or during the iteration, we I mean that is how this trace option is very helpful particularly when there you feel there are lot of you know components which is in very minuscule amount.

So, we do not worry about the convergence of those you know minuscule amount of the components and we you know focus more on the you know the primary components. Of course or you can have this you know option default option is thresholding but you can also have that option to have you know gradual thresholding like you know with the value of the tolerance or sorry not with the tolerance with the value of the this mass fraction you can decrease the threshold value.

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Convergence Methods.

Tear Convergence.

↳ Wegstein (default).  
Direct.  
Broyden.  
Newton.

So, that is the gradual method. What about the convergence methods? So, the convergence methods have the following options. So, you have the tear convergence. So, there are other field also like the design specification you know optimization etcetera but we are more worried about the tear convergence. So, the different you know these options or the I would

say the algorithms that is present are Wegstein, then you have the Direct, then you have the Broyden method and you have the Newton method this is the default method.

So, what are the differences. So, in this Wegstein method is actually the quickest that is one of the biggest advantage, and you know this interaction between the variables is essentially ignored. So, that is the (I mean) case when the variables are strongly coupled it does not work well and this is based on the extrapolation of the direct or direct substitution iteration. Next is the Direct method this is a very slow method but you get more chances of success.

So, the new value of the tear stream in this Direct method is the value resulting from the previous flowsheet calculation pass. So, this is definitely a you know better than the Wegstein method and it also helps you to pinpoint the actual problem and this is more stable compared to the Wegstein method. So, this is easy to identify convergence problem such as if there is component buildup in the system etcetera.

Broyden method is actually faster but it is not so reliable and this is not something I would recommend actually. So, this method is an approximation or a linearization of the Newton method and this is useful I mean this sometimes is useful as well as this is true for the Newton method also when there is the when this tear variables that are quite interdependent or there are recycling loops present in the system and this interrelation or the nesting is very important.

Newton method is again modification it is essentially the newton you know method of simultaneous non-linear equations or essentially the sort of in simultaneous correction equations form and this is particularly reliable when you have recycling streams, of course one should try the Broyden method for first that is the linearization version or the approximate linearized version of the Newton method but if the Broyden method does not work then you should go for the Newton method.

So, newton method for tear streams only works best when the number of components is small and only when convergence cannot be achieved by other methods. So, this is the one of the most reliable methods but this is very slow and when you do not have too many number of streams in the system. So, this is about the different convergence you know methods that is present here and we will see them in the in the software block in the convergence method block let us go to the software platform.

(Refer Slide Time: 35:26)



Simulation 4.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

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

Main Flowsheet: 1 (MATERIAL) Results Summary - Run Status Control Panel

Simulation calculations completed ...

\*\*\* No Warnings were issued during Input Translation \*\*\*

\*\*\* Summary of Simulation Errors \*\*\*

	Physical Property	System	Simulation
Terminal Errors	0	0	0
Severe Errors	0	0	0
Errors	0	0	2
Warnings	0	0	1

Generating results ...

<< Run Saved >>

<< Run Saved >>

<< Run Saved >>

<< Run Saved >>

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

Material, Pump, Compr, MCompr, Valve, Pipe, Pipeline

16:44 06-04-2022

Simulation 4.apwz - Aspen Plus V8.8 - aspenONE

File Home Economics Dynamics Equation Oriented View Customize Resources

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

Main Flowsheet: Control Panel Options

Tear Convergence: Default Methods Sequencing Information

Tear stream convergence parameters

Tolerance: 0.0001

Trace threshold: [ ]

Trace option: Cutoff

Component group: [ ]

State: Pressure & enthalpy

Restore tears on error

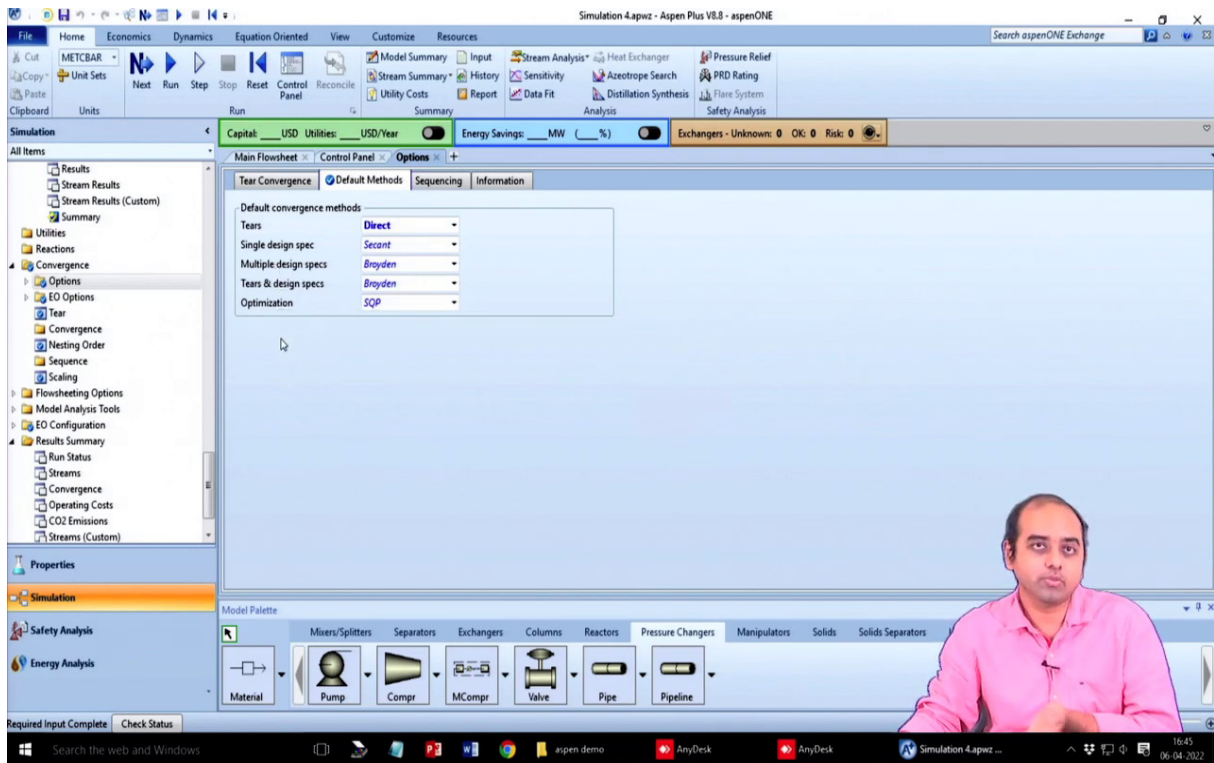
Flash tear streams

Iteration History: Display: Maximum error / tolerance

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

Material, Pump, Compr, MCompr, Valve, Pipe, Pipeline

16:44 06-04-2022



So, here we got the error and we understood that it is because of some mass balance issue in the recycling stream and you know the recycling stream is essentially the tear stream in this case. So, we go to the convergence block we go to the options you see that in the options it is written that the tear convergence is 0.001 trace thresholding cutoff etcetera is there all default options are provided if you want to change the default you play place your trace threshold or by default it is the you know tolerance by thousand sorry by hundred then about the Default method.

So, this is regarding the tear variable see by default the Wegstein method is selected. So, apart from using the Wegstein method let us use the Direct method and see whether it works or not. Let us save it let us try to reset because we have changed the default setting other you know these criteria of design specification options etcetera is not applicable in our problem. So, we do not worry about those methods.

(Refer Slide Time: 36:38)

The screenshot shows the Aspen Plus V8.8 software interface. The main window displays the 'Options' tab for 'Tearing and sequencing parameters'. The parameters are as follows:

- Design spec nesting: Inside
- User nesting: Outside
- Variable weight: 1
- Loop weight: 1
- Tear Calculator export variables:
- Check sequence:
- Use affected block logic:

The interface also shows a 'Model Palette' at the bottom with various process units like Material, Pump, Compr, MCompr, Valve, Pipe, and Pipeline. A person in a pink shirt is visible in the bottom right corner of the screen.

The screenshot shows the Aspen Plus V8.8 software interface with a 'Simulation Errors' dialog box open. The dialog box contains the following text:

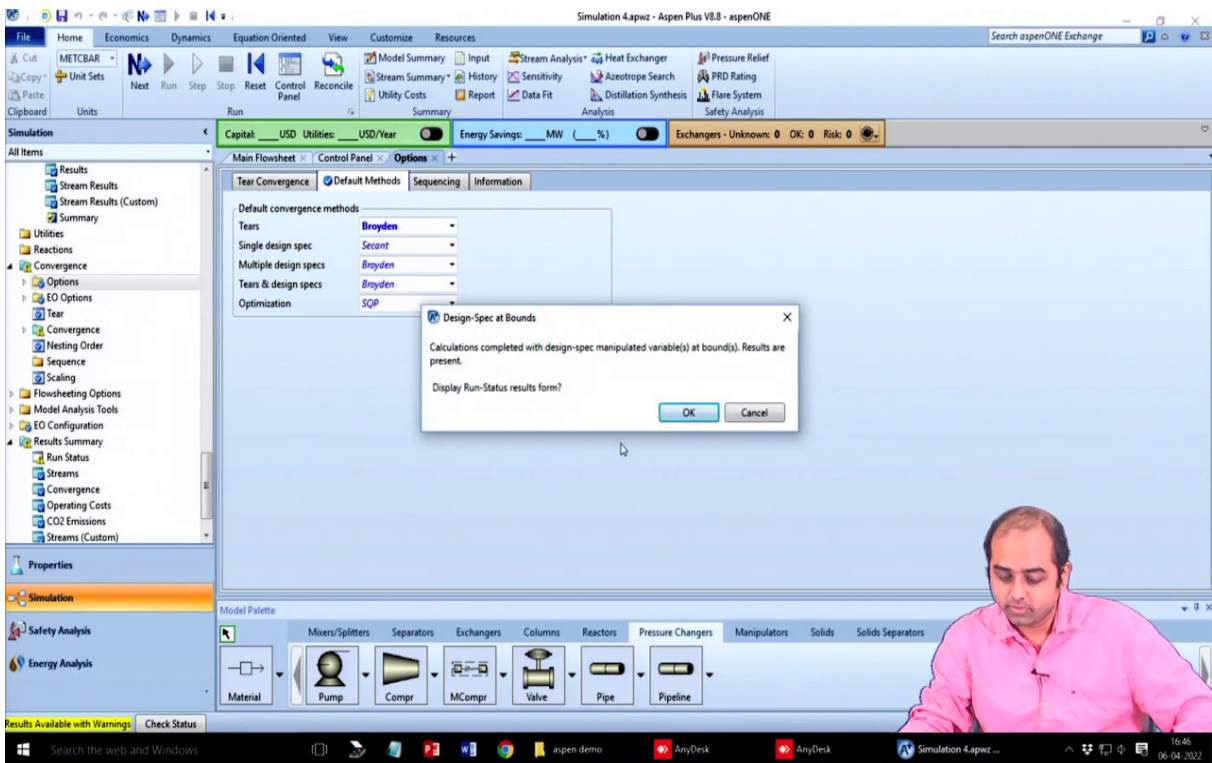
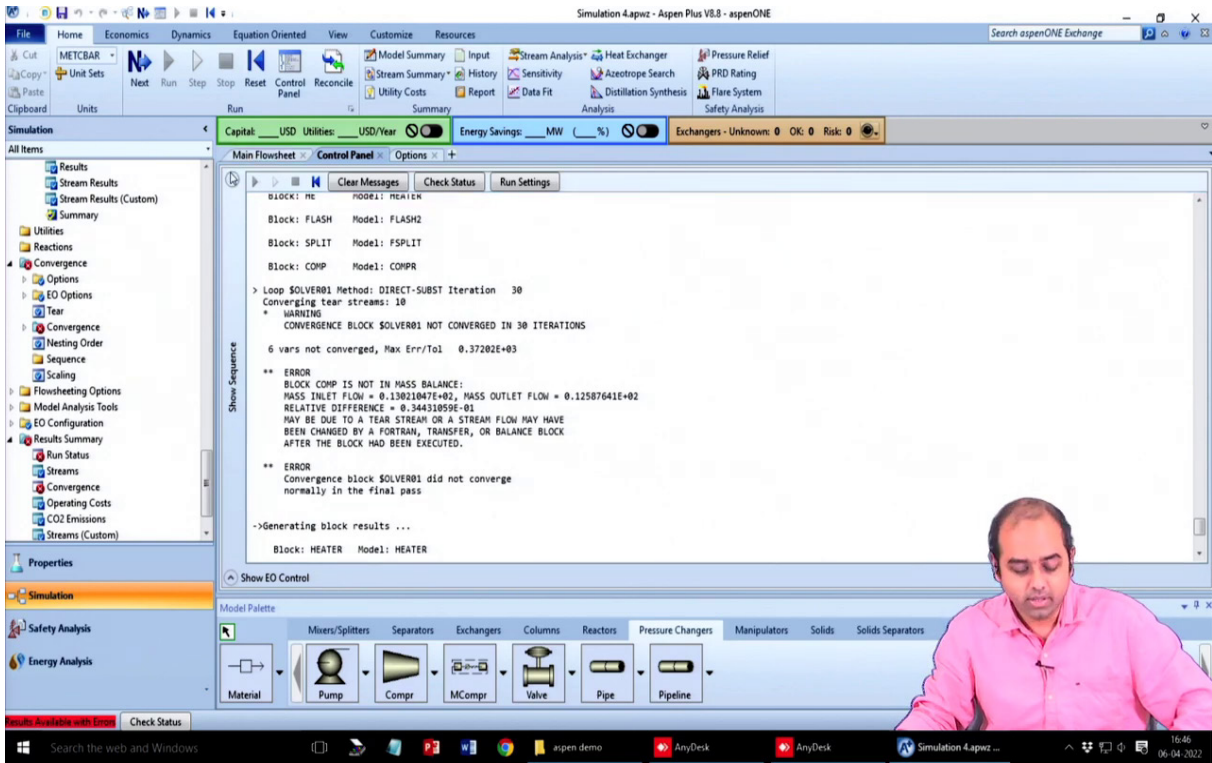
Your simulation has completed with errors. Results are present.

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

The background window shows the 'Options' tab for 'Tearing and sequencing parameters' with the following settings:

- Tolerance: 0.0001
- Trace threshold: [empty]
- Trace option: Cutoff
- Component group: [empty]
- State: Pressure & enthalpy
- Restore tears on error:
- Flash tear streams:
- Iteration History: Display Maximum error / tolerance

The 'Simulation Errors' dialog box has 'OK' and 'Cancel' buttons. A person in a pink shirt is visible in the bottom right corner of the screen.



The third block was sequencing and the sequencing is by default we do not change them it is all inside from the inside it starts and then moves to the recycling stream let us run it and see whether still we face the problem your solution simulation has been completed with errors. So, let us see the control panels.

So, even after 30 iterations we see that the relative difference is not below the tolerance for the tear stream in this case is the late cycling stream and the problem was still there with the compressor block. So, so again we try the third option. So, one thing we can try we already know that the you know the default value is 0.03.

(Refer Slide Time: 37:49)

*** Summary of Simulation Errors ***			
	Physical Property	System	Simulation
Terminal Errors	0	0	0
Severe Errors	0	0	0
Errors	0	0	0
Warnings	0	0	1

So, I mean let us try the other options first, Broyden method. So, reset let us try to run it. So, it shows a warning. So, now the error has gone and it completed with warning. So, what is the warning. So, if you see that it says that streams crossing the loop converged by solver block are not in mass balance. So, there is again the same block that compressor block on the recycling stream but the relative difference is significantly low now it is just close to the tolerance.

So, the imbalance may be due to the large recycle flow and a relatively loose tear stream tolerance. So, to avoid this relative difference I mean the relative difference is now point double zero I mean 0.00014. So, it is just close to tolerance that is why it is saying that this is a warning that even though you are close to convergence even though you are close to convergence but still you know there may be even for the full convergence has not been achieved but you are almost close to the convergence for a particular stream.

So, we are we have the results it may not be entirely you know accurate but we have the results. So, what we can do is that in the options we can alter the tear tolerance reduce it to 0.001. So, it will satisfy now of course this is not a correct way I mean we should have a much stricter tolerance but since this is finding it difficult we relax the tolerance criteria a little bit.

(Refer Slide Time: 39:12)

The screenshot displays the Aspen Plus V8.8 software interface. The main window is titled "Simulation 4.apwz - Aspen Plus V8.8 - aspenONE". The "Options" tab is active, showing "Tear Convergence" parameters. A dialog box titled "Design-Spec at Bounds" is open, displaying the message: "Calculations completed with design-spec manipulated variable(s) at bound(s). Results are present." and "Display Run-Status results?". The interface includes a menu bar, a toolbar, a left-hand navigation pane, and a bottom status bar. A person in a pink shirt is visible in the bottom right corner of the frame.

The screenshot displays the Aspen Plus V8.8 software interface, showing the "Results Summary - Run Status" window. The window contains sections for "Convergence status", "Property status", and "Aspen Plus messages". The "Aspen Plus messages" section displays the text: "The following Convergence blocks were completed with warnings: SOLVERB1". The interface includes a menu bar, a toolbar, a left-hand navigation pane, and a bottom status bar. A person in a pink shirt is visible in the bottom right corner of the frame.

Simulation 4.apwz - Aspen Plus V8.8 - aspenONE

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

Convergence status  
Block calculations were completed with warnings

Property status  
Property calculations were completed normally

Aspen Plus messages:  
 \* WARNING: STREAMS CROSSING THE LOOP CONVERGED BY SOLVER01 ARE NOT IN MASS BALANCE:  
 MASS INLET FLOW = 0.43470803E+00, MASS OUTLET FLOW = 0.43464675E+00  
 RELATIVE DIFFERENCE = 0.14100969E-03  
 IMBALANCE MAY BE DUE TO A LARGE RECYCLE FLOW, AND A RELATIVELY LOOSE TEAR STREAM TOLERANCE.

Model Palette: Material, Pump, Compr, MCompr, Valve, Pipe, Pipeline

Simulation 4.apwz - Aspen Plus V8.8 - aspenONE

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

Tear Convergence Default Methods Sequencing Information

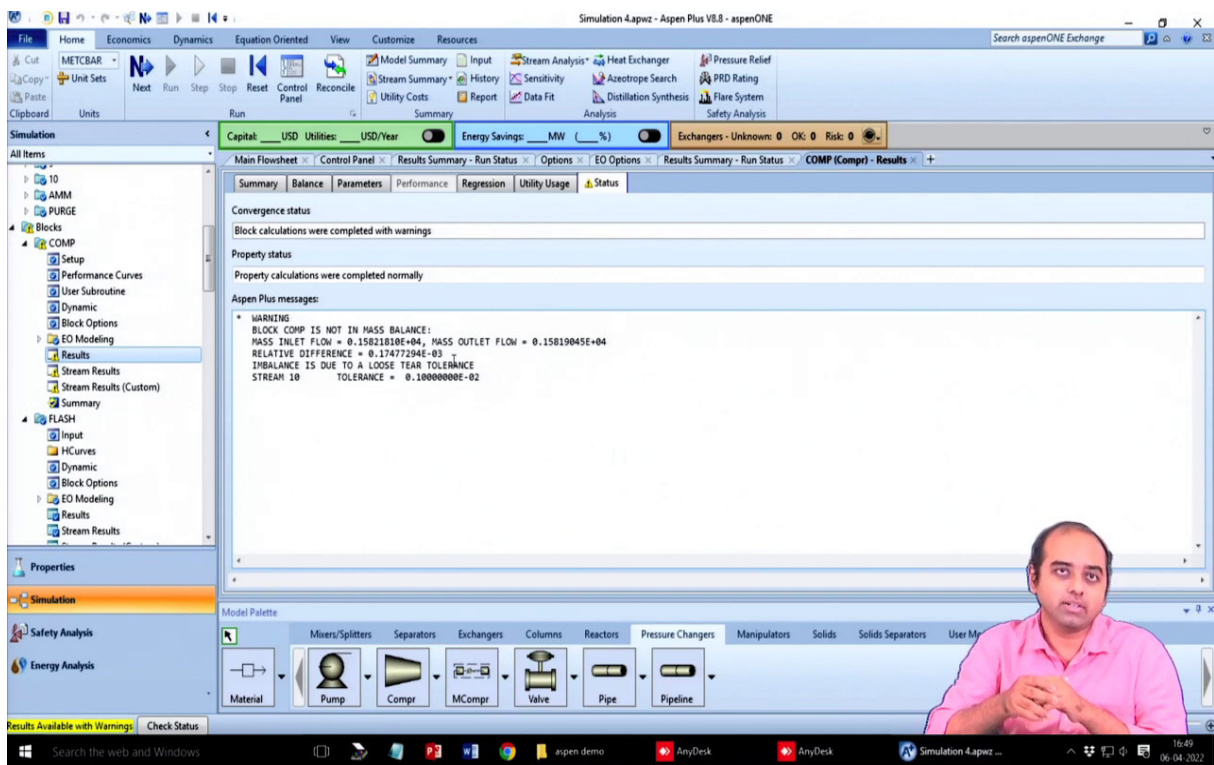
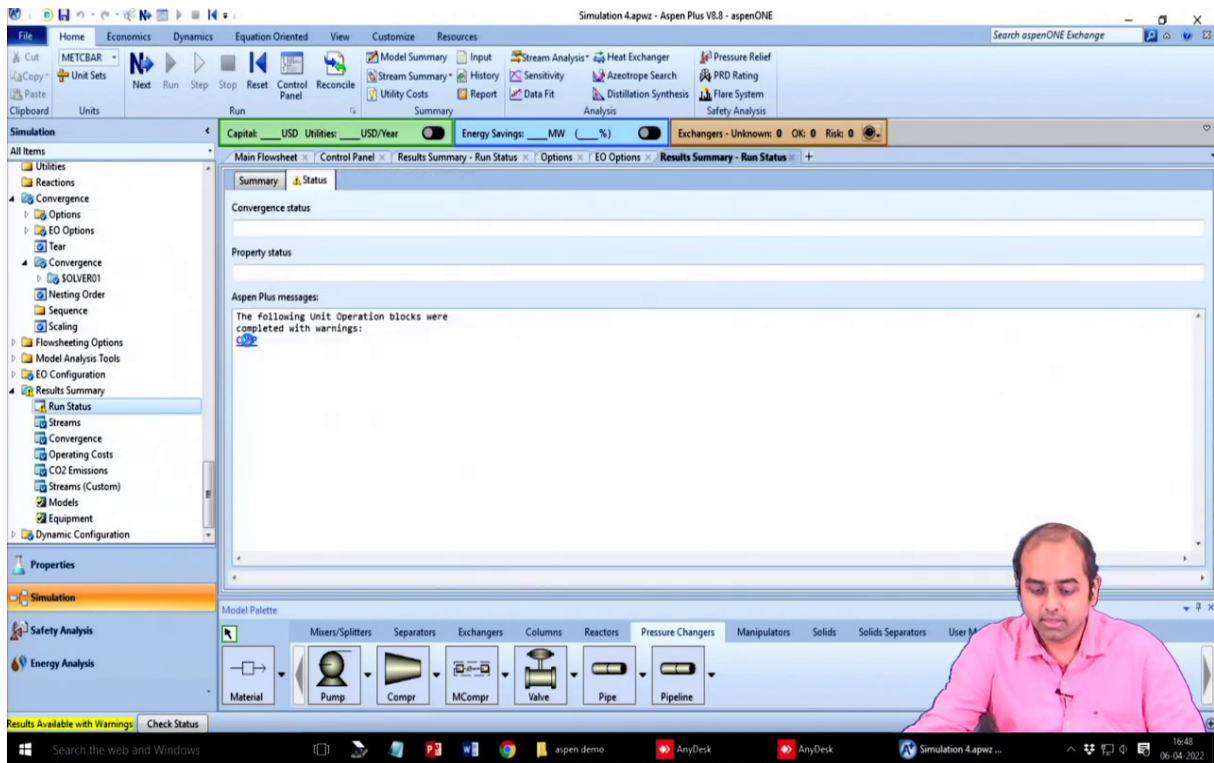
Default convergence methods  
 Tears: Newton  
 Single design spec: Secant  
 Multiple design specs: Broyden  
 Tears & design specs: Broyden  
 Optimization: SQP

Simulation Warnings  
 Your simulation has completed with warnings.  
 Results are present.

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

Model Palette: Material, Pump, Compr, MCompr, Valve, Pipe, Pipeline



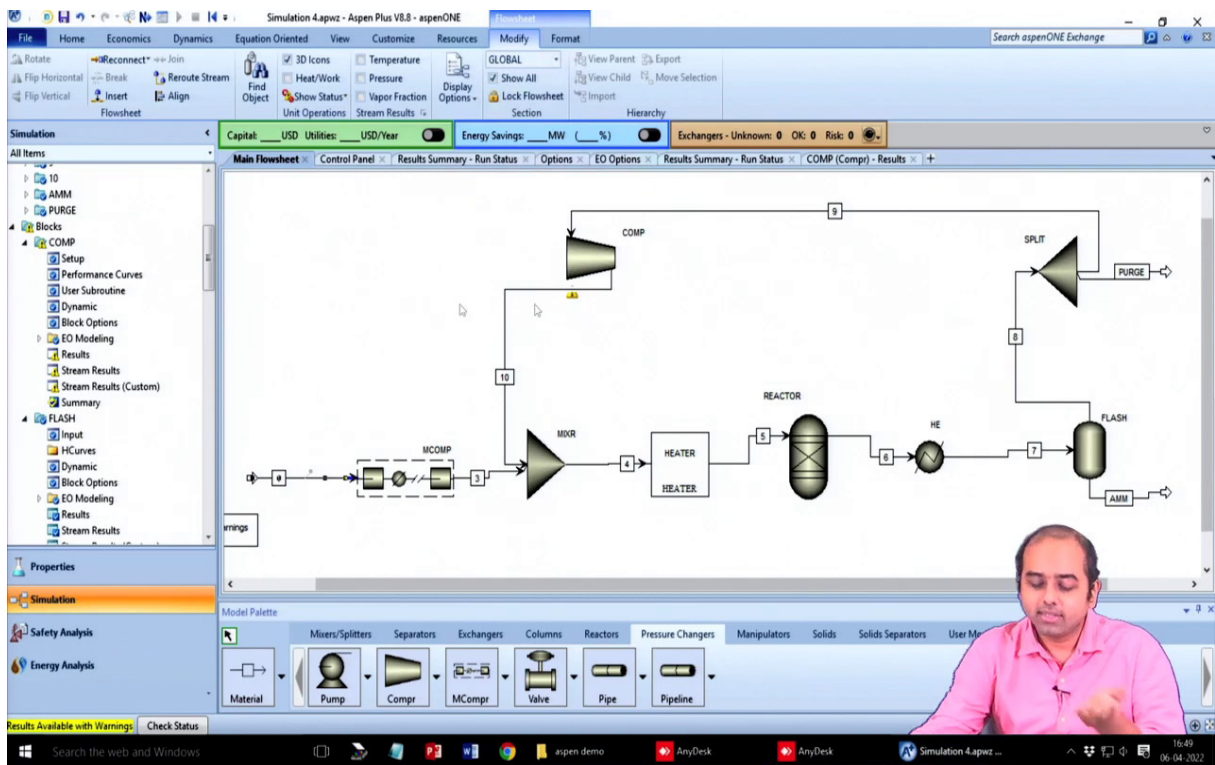


So, we reset and then we try to run it. So, again it says that results are available but there are issues with the tolerance. So, even though the tolerance is achieved that is why our warning is there we are getting some difference. So, let us try the last one last option sorry convergence option, Default method from Broyden to Newton reset the calculations once again and let us

try to run it. So, even with the Newton method also still these warnings are there but here also we see that the relative difference is below the tolerance.

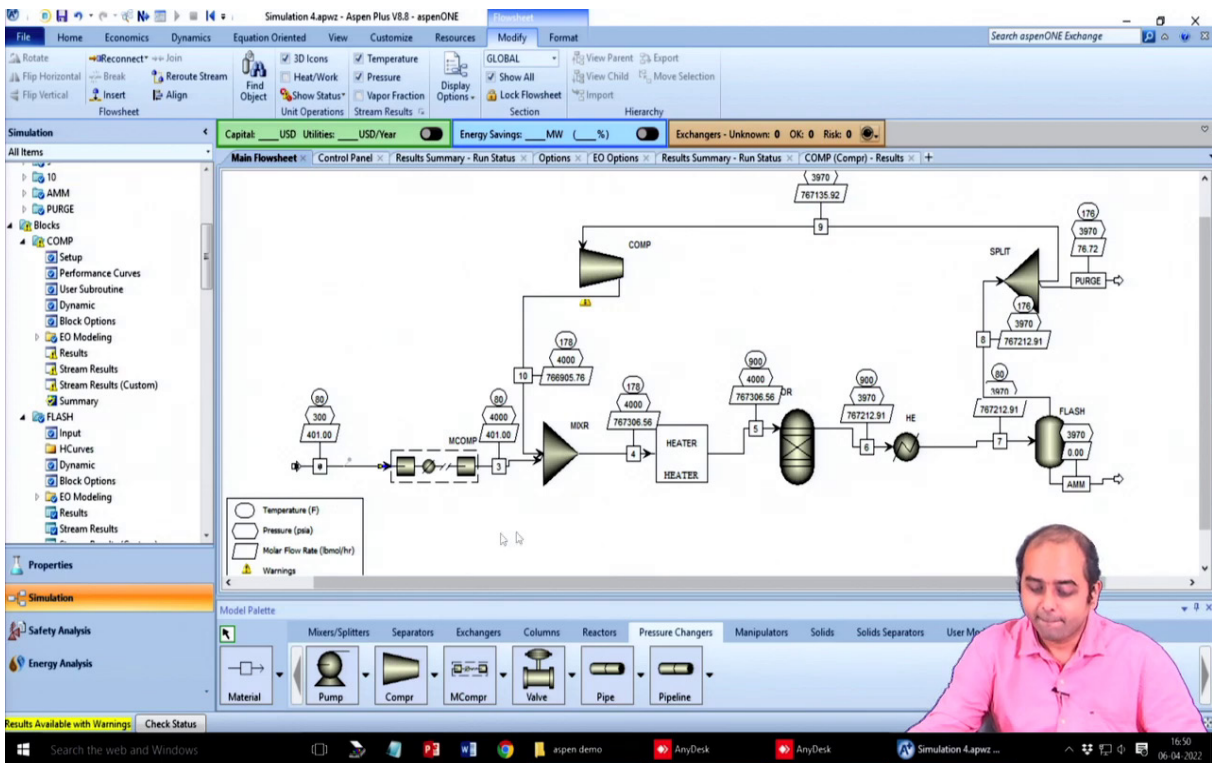
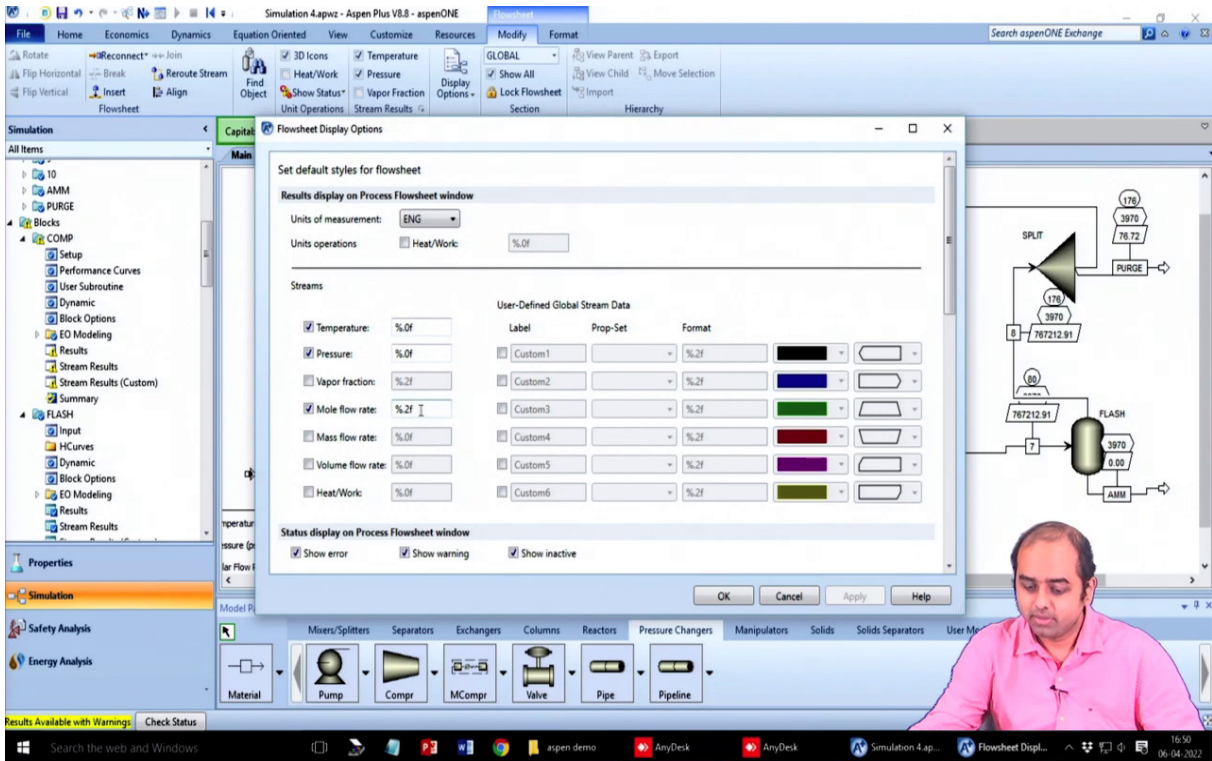
So, this tells you that how the. So, the first settings or the direct method actually failed to compute this at all but the Broyden and the Newton method were actually successful in getting you know achieving the tolerance set by us and tolerance 10 to the power minus 4 is actually too strict. So, we may need to relax it little bit to 10 to the power minus 3 to achieve this convergence.

(Refer Slide Time: 40:34)



The screenshot displays the Aspen Plus V8.8 simulation environment. The main window shows a process flow diagram with the following units: COMP (Compressor), MIXER, HEATER, REACTOR, HE (Heat Exchanger), FLASH, and AMM (Amine Mixture). The process starts with a feed stream (27) entering a MIXER, followed by a HEATER, a REACTOR, another HEATER, and a FLASH unit. A COMPRESSOR (COMP) is connected to the process. The diagram includes stream numbers (e.g., 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100) and stream names (e.g., PURGE, AMM). The interface includes a menu bar (File, Home, Economics, Dynamics, Equation Oriented, View, Customize, Resources, Modify, Format), a toolbar with various simulation options, and a sidebar with simulation options (Simulation, Safety Analysis, Energy Analysis). The status bar at the bottom shows the system tray and the date 06-04-2022.

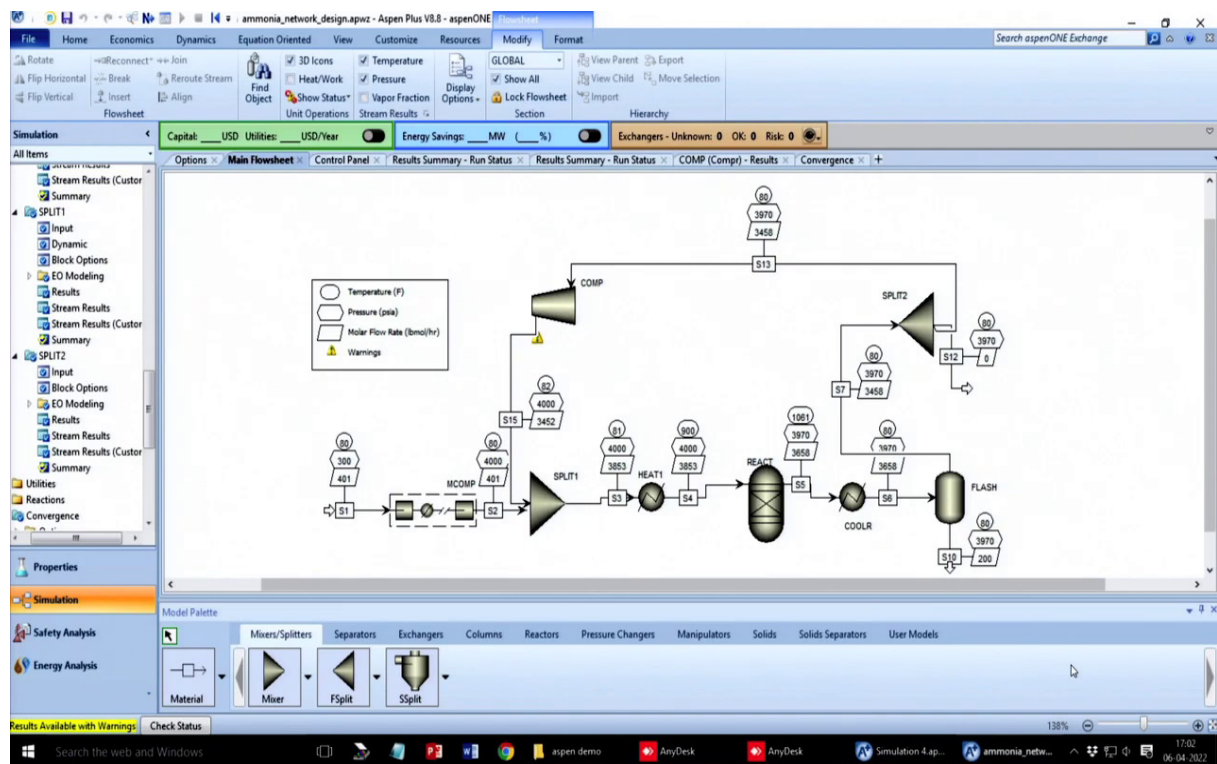
The screenshot displays the Aspen Plus V8.8 simulation environment. The main window shows a process flow diagram with the following units: COMP (Compressor), MIXER, HEATER, REACTOR, HE (Heat Exchanger), FLASH, and AMM (Amine Mixture). The process starts with a feed stream (27) entering a MIXER, followed by a HEATER, a REACTOR, another HEATER, and a FLASH unit. A COMPRESSOR (COMP) is connected to the process. The diagram includes stream numbers (e.g., 21, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100) and stream names (e.g., PURGE, AMM). The interface includes a menu bar (File, Home, Economics, Dynamics, Equation Oriented, View, Customize, Resources, Modify, Format), a toolbar with various simulation options, and a sidebar with simulation options (Simulation, Safety Analysis, Energy Analysis). The status bar at the bottom shows the system tray and the date 06-04-2022.



So, now let us go to the main flow sheet and so this warning sign is given and try to see I mean try to you know display the different stream properties for example temperature pressure let us define the mole flow rate apply. So, as you can see because of this slight issue in the tolerance this is slightly imbalanced. So, the input to the compressor is 767135 whereas the output is 766905.

So, it is not entirely same because of this issue but this is a very small amount the relative difference is very small actually for which the solution actually gave this warning to us and the rest of the calculations are pretty fine and you can see that convergence is achieved almost everywhere there is no warning the molar flow rate is mentioned here is pound mole per hour.

(Refer Slide Time: 42:03)



So, this is the display of the final flow sheet and all the stream properties as you can see can be also plotted in the flow sheet itself as a complete PFD diagram and this is something I found it quite useful rather than plotting down the individual streams of course if you look want to look into the details about how much is the conversion or how much is the ammonia or the hydrogen molar flow rate you can of course look into the individual streams and find out that what are the relative you know what is the amount of the output that we are getting from the system what is the ammonia output and everything.

So, I think this is all that I have to say regarding the software demonstration there are several you know such similar problems or tutorials which are available online I encourage all of you to you know try to work them out yourself try to learn more about them, try there are some more things that could be done using the software for example something known as the design specification.

So, by the design specification you can actually work out the inverse problem, if I try to select let us say I want the final output to be this value then what is the possible you know value of one of the process parameters that we need to determine can be actually solved from the this design specification.

So, it is not the sensitivity but we specify a variable which we want to alter. So, that the desired value of a final target product is attained similarly you can do the you know cost optimization energy analysis and all further calculations complex calculations can also be done for a process flow sheet.

So, I hope all of you have learnt some you know idea regarding the software and how to use it and what are the is usefulness and where the strengths and the limitations I hope all of you will found it quite useful in your career I mean the software use in your career in some with something or the other related to process design and simulation. Thank you and see you everyone in the next week.