PROCESS SIMULATION LAB

Day 4
Group 2

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Submission Date

13/09/2023

Question 2

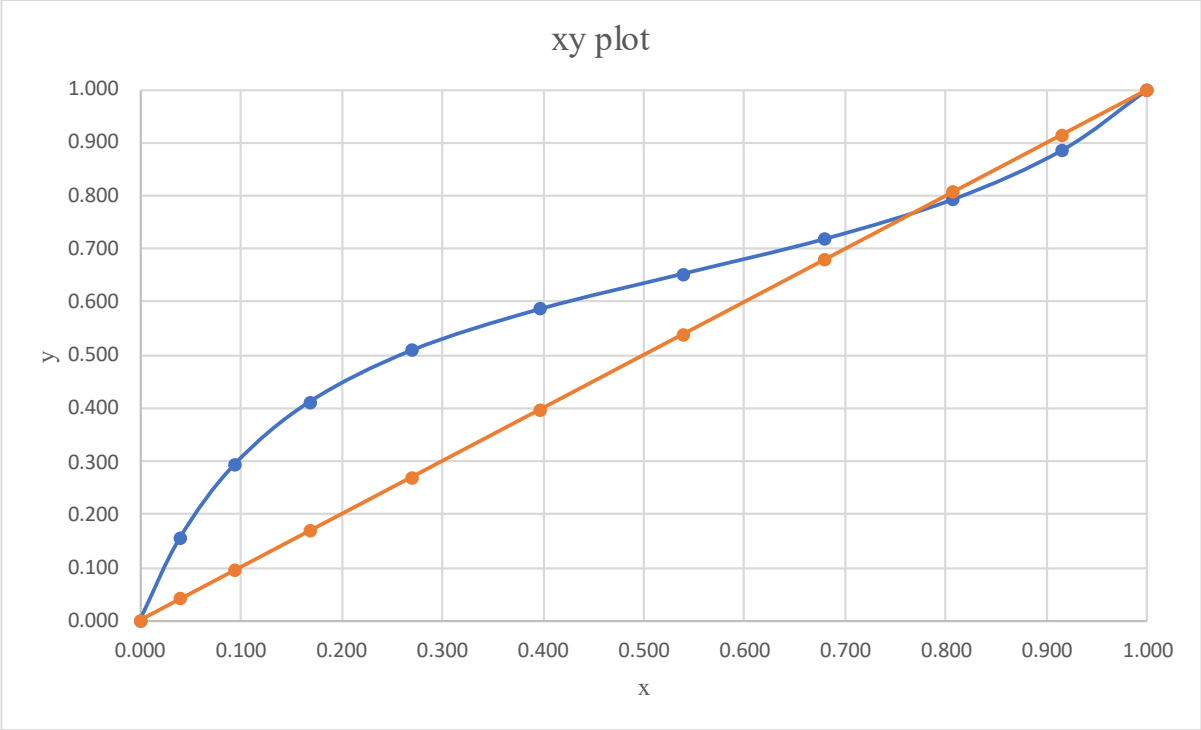
Using ASPEN Hysys to a create VLE diagrams (xy, T–xy) diagrams for a binary mixture of di-isopropyl ether and 2-propanol at atmospheric pressure. Use Wilson equation of state for the liquid phase and Peng - Robinson equation of state for the vapour phase property prediction.

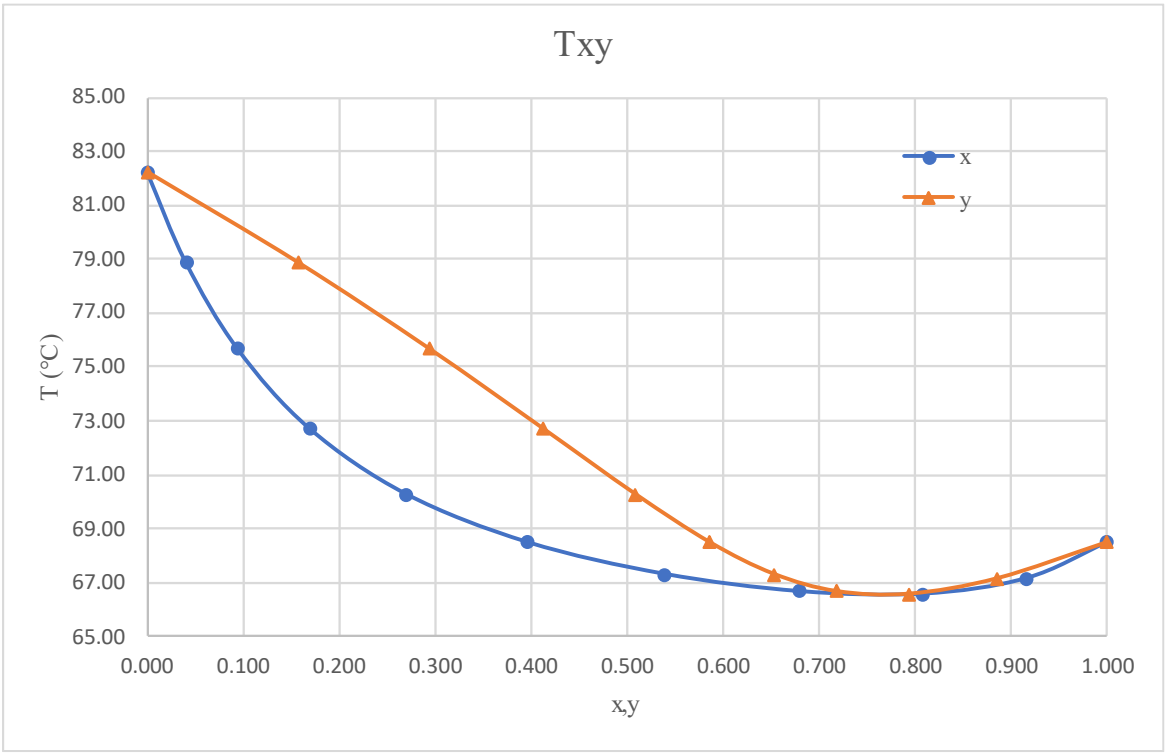
Answer

VLE Data for the binary mixture of di-isopropyl ether and 2-propanol

Case	Ether-Molar Flow [kg mole/h]	Mixture Temperature [C]	Mole Fraction (Liquid Phase Ether)	Mole Fraction (Vapour Phase Ether)
Case 1	0.000	82.25	0.000	0.000
Case 2	0.200	78.90	0.040	0.156
Case 3	0.400	75.66	0.094	0.294
Case 4	0.600	72.71	0.169	0.412
Case 5	0.800	70.27	0.270	0.508
Case 6	1.000	68.47	0.397	0.586
Case 7	1.200	67.30	0.538	0.652
Case 8	1.400	66.65	0.679	0.718
Case 9	1.600	66.56	0.807	0.793
Case 10	1.800	67.14	0.915	0.886
Case 11	2.000	68.48	1.000	1.000

VLE Diagrams:

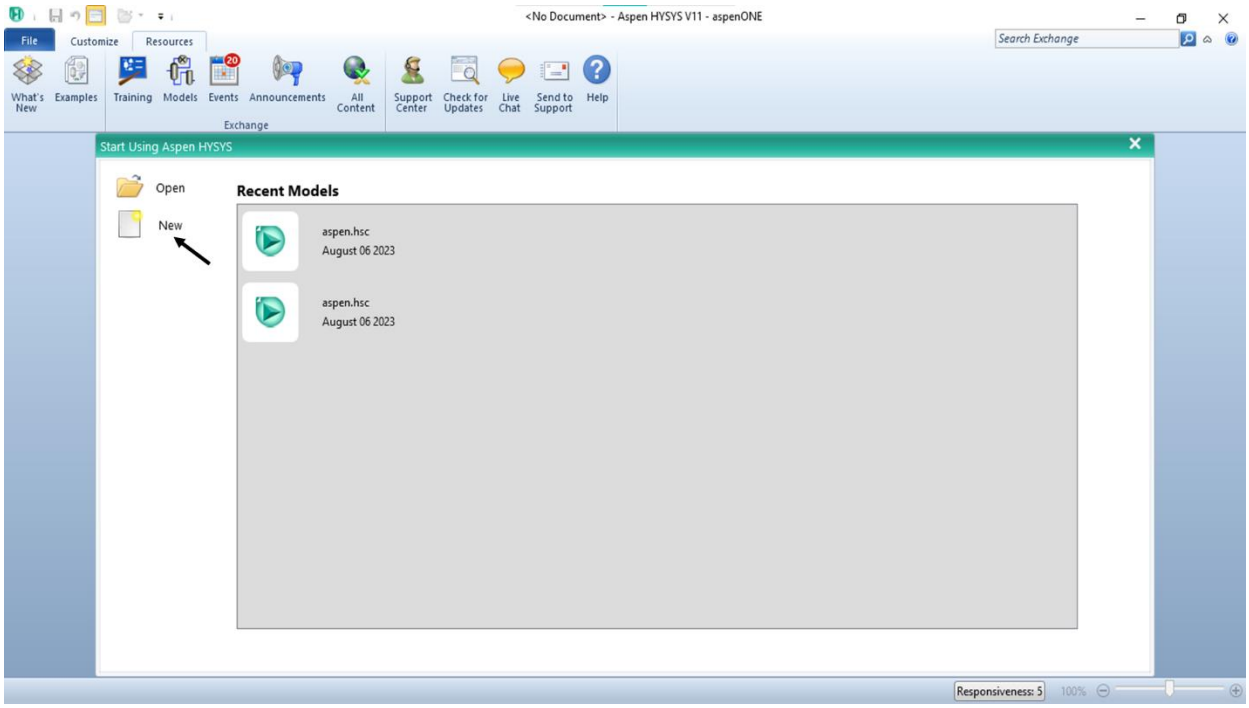




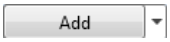
Steps to solve the questions are as follows:

Step 1:

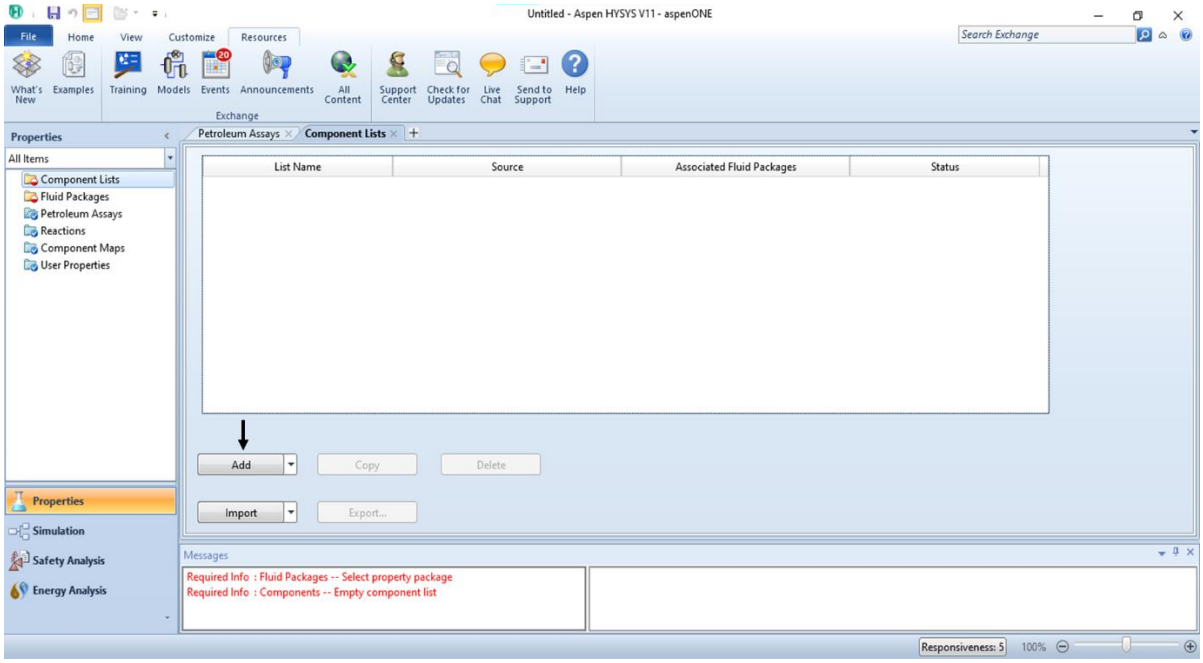
At first, we ASPEN HYSYS software by clicking on the shortcut icon from the desktop. The Initial Layout looks like the following. From the New menu we clicked on button to create a blank Simulation Workbook page.



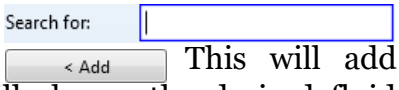
Step 2:

Now in the next page we will click on 

icon to select the components required for our simulation. Here we are dealing only with water we will add only water.



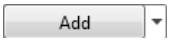
Step 4:

Now in the Component list page we will search in the box. Then we will select the benzene & toluene and click. 

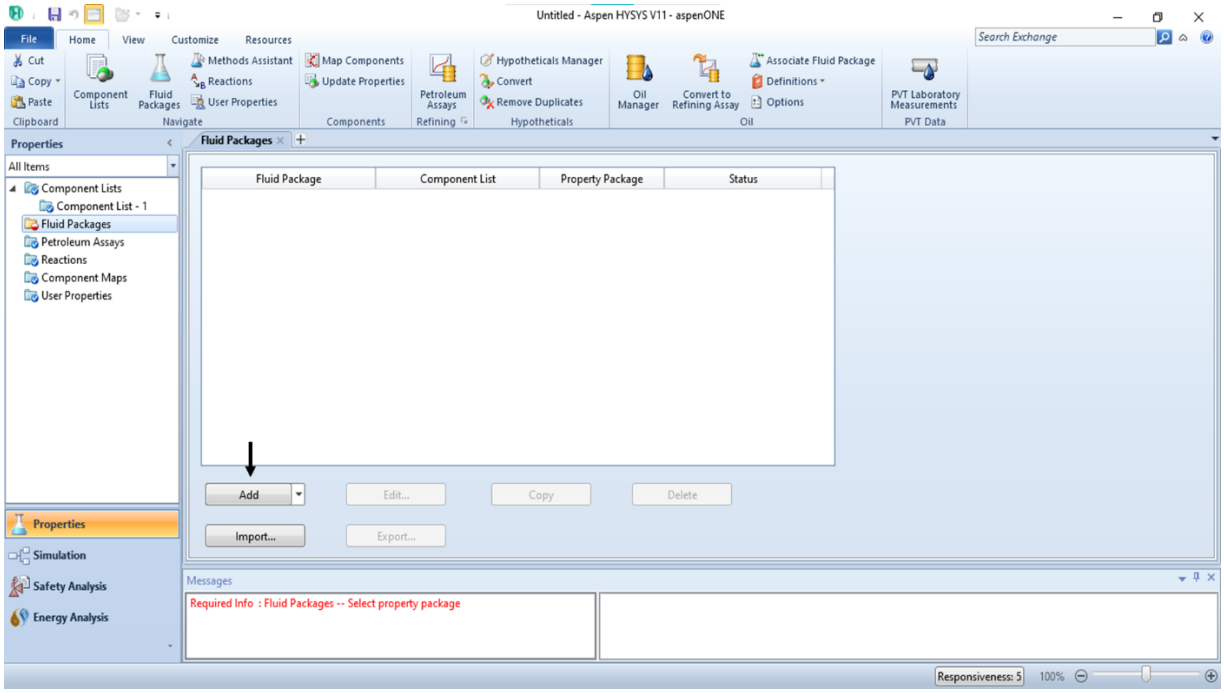
This will add benzene & toluene in the component list. Now we will choose the desired fluid packages by clicking on

icon.

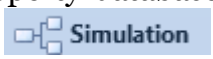
Step 5:

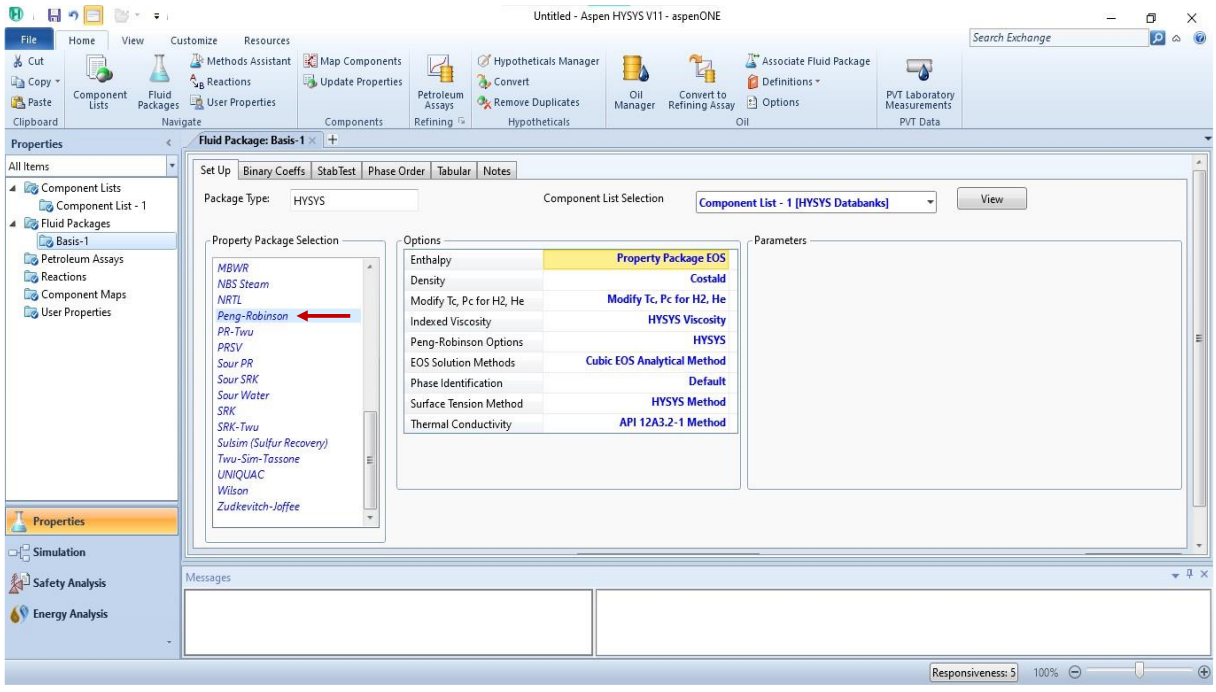
In the Fluid Packages tab, we will click 

to add new fluid packages.



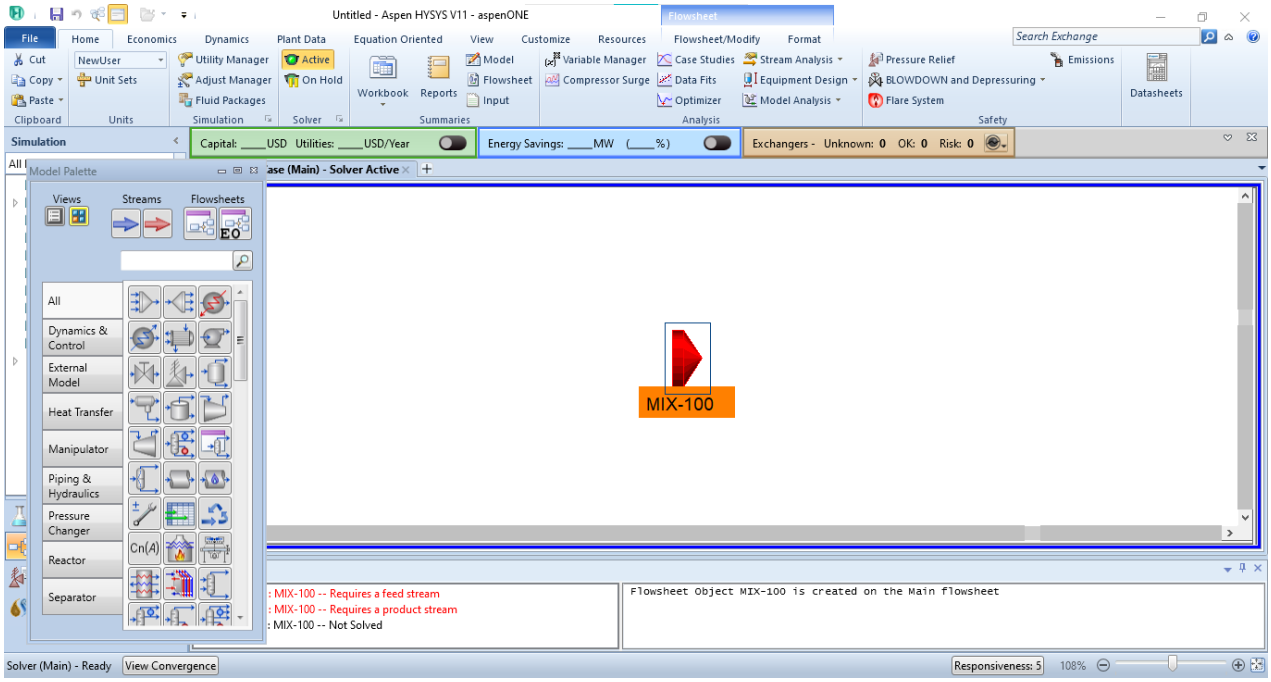
Step 6:

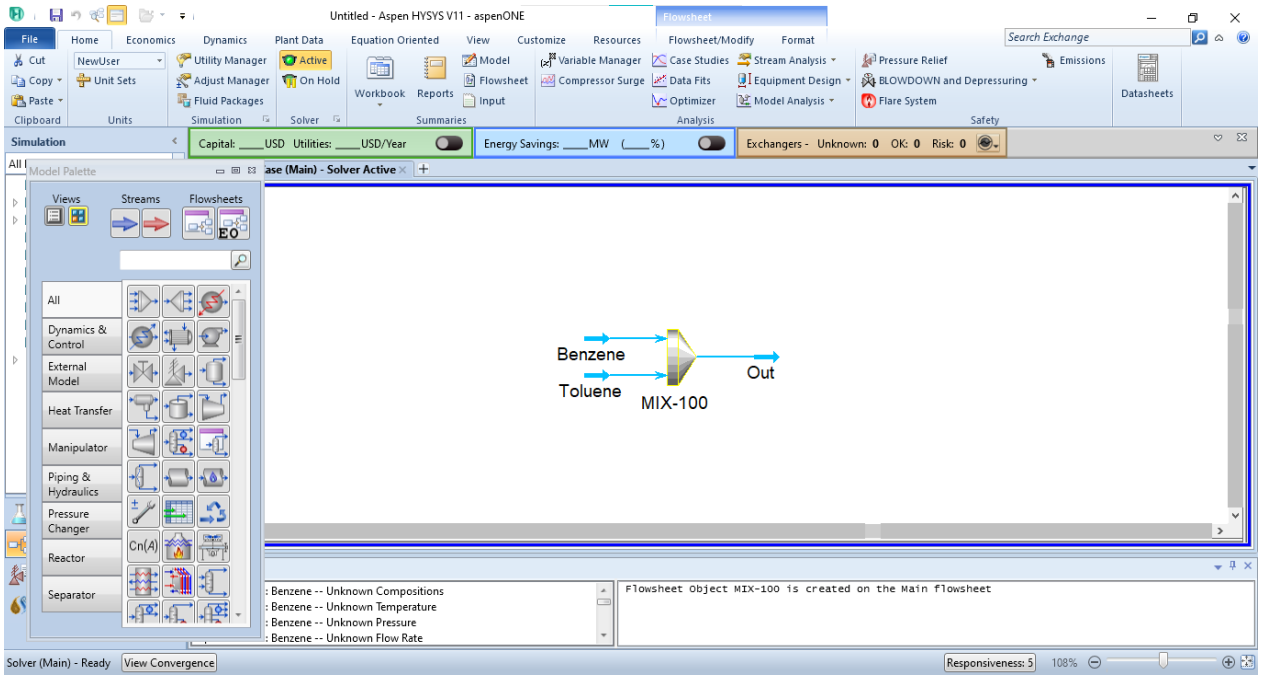
According to our given problem, we are supposed to use Peng-Robinson package for our problem. So, from the dropdown menu, we will select the Peng-Robinson option. Now our components and property databases are ready. We are ready to move to Simulation Tab by clicking  the button.



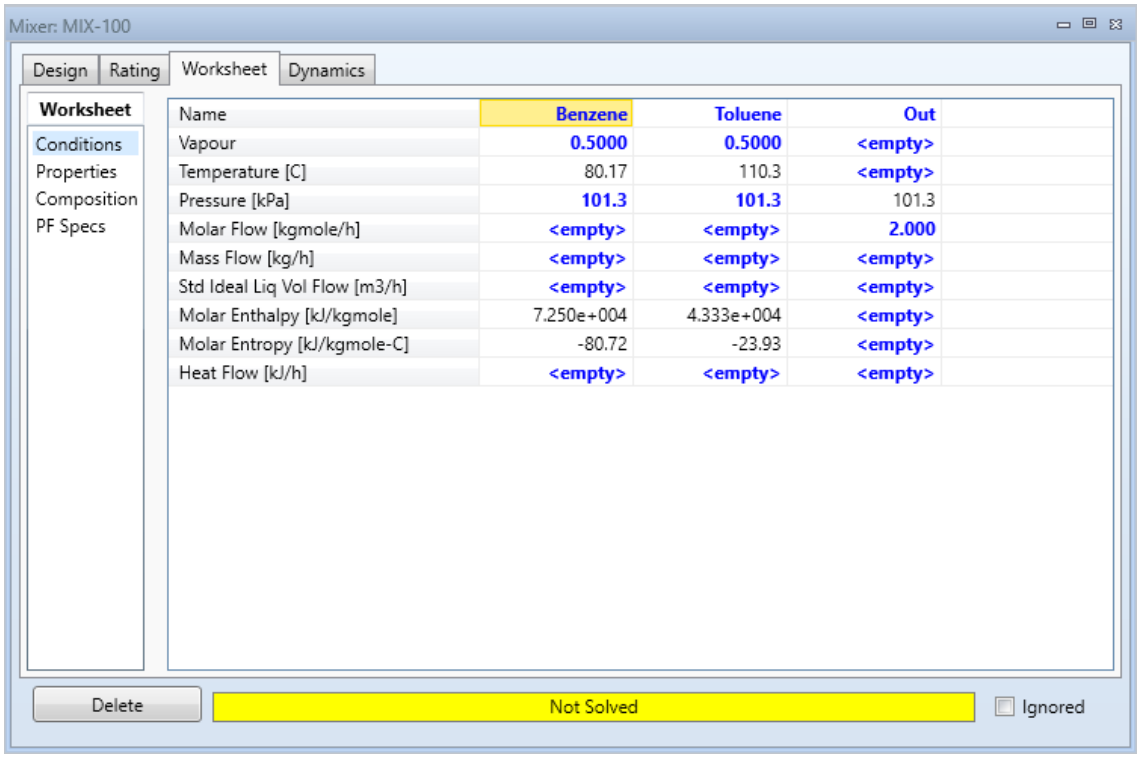
Step 7:

This is the most important step. First, we will drag a Mixer and drop it to the blank space. Now we will name all the connected streams required for this problem. Now, we need to input all the given data for the problem.

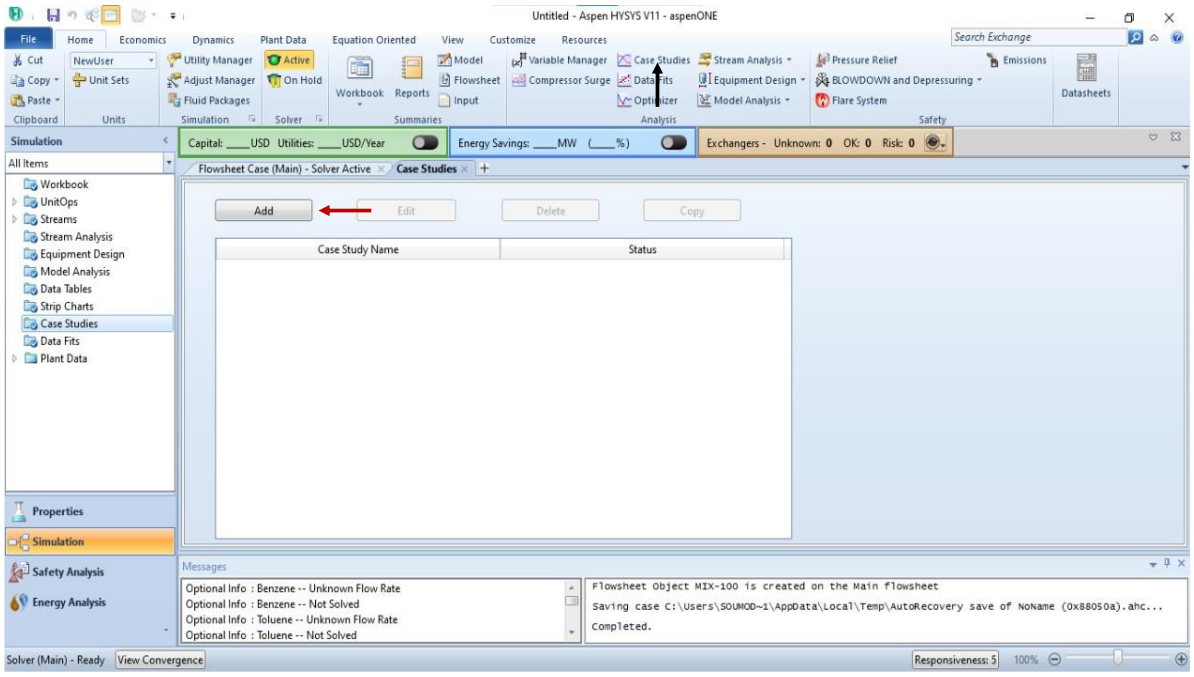




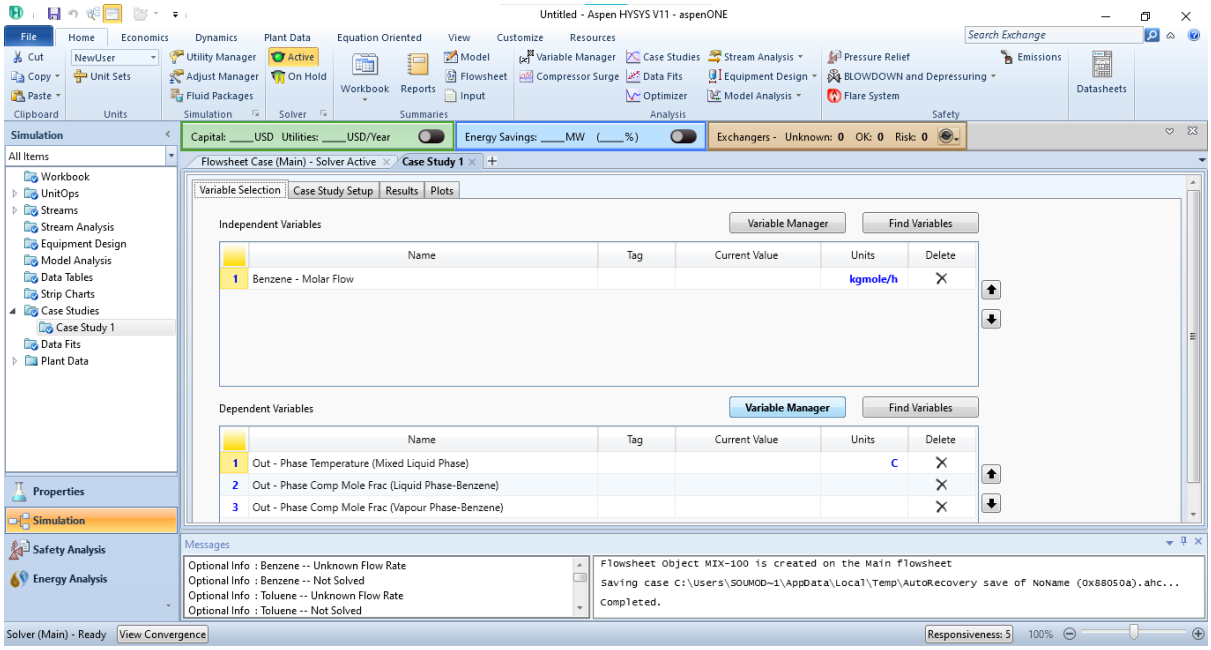
After clicking on the mixer, we will click on tab which will open another dialogue where we can enter the inlet and outlet stream properties Worksheet according to the given problem statements. Here as the mixture is a binary mixture, we will assume that the benzene and toluene both are entering at 50 % vaporised conditions. Also, the total outlet molar flowrate is constant at 2 $kgmole/hr$.



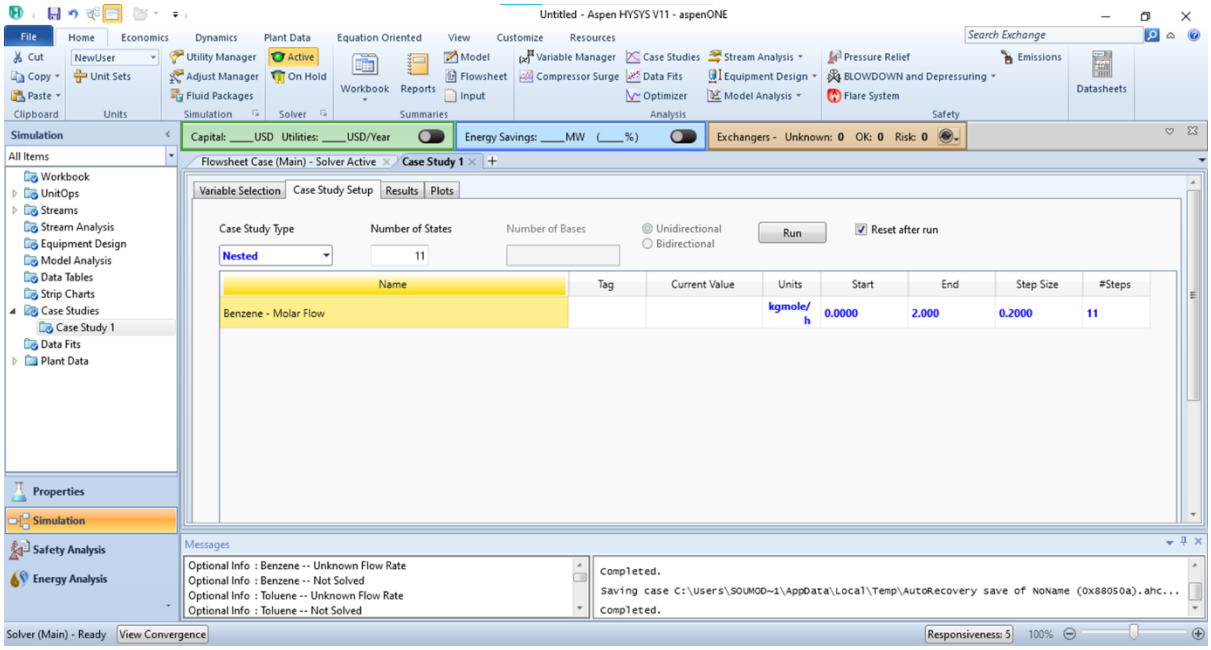
We can observe that some important data (e.g. Molar Flowrates) are missing from the worksheet. So now we will use the Case Study tool to generate the equilibrium data for different flow rates of benzene.

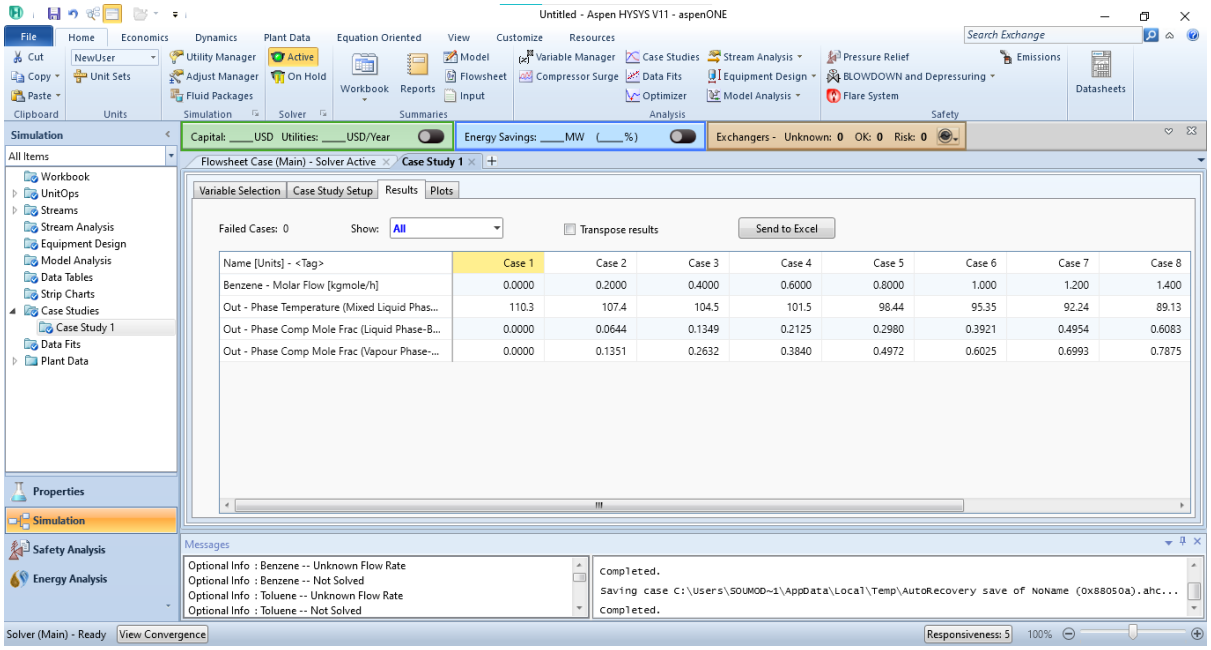


After clicking on the Add button, we will add the dependent and independent variables for the system. In the given system, independent variable is Molar flowrate of benzene and Dependent variables are Mixture Temperature, Liquid Phase and Vapour Phase mole fraction of Benzene.



Now we will click on the Case Study Setup button. Here we will mention the start point as 0 and end point as 2 with step size 0.2 $kgmole/hr$. After that we will click on the Run button to generate the VLE data. Then this data is exported to excel to generate the plots mentioned earlier.




Untitled - Aspen HYSYS V11 - aspenONE
File
Home
Economics
Dynamics
Plant Data
Equation Oriented
View
Customize
Resources
Search Exchange
Cut
Copy
Paste
Clipboard
NewUser
Unit Sets
Units
Utility Manager
Adjust Manager
Fluid Packages
Simulation
Active
On Hold
Solver
Workbook
Reports
Model
Flowsheet
Input
Summaries
Variable Manager
Compressor Surge
Case Studies
Data Fits
Optimizer
Stream Analysis
Equipment Design
Model Analysis
Analysis
Pressure Relief
BLOWDOWN and Depressuring
Flare System
Emissions
Safety
Datasheets
Simulation
All Items
Workbook
UnitOps
Streams
Stream Analysis
Equipment Design
Model Analysis
Data Tables
Strip Charts
Case Studies
Case Study 1
Data Fits
Plant Data
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Exchangers - Unknown: 0 OK: 0 Risk: 0
Flowsheet Case (Main) - Solver Active
Case Study 1
Variable Selection
Case Study Setup
Results
Plots
Failed Cases: 0
Show: All
Transpose results
Send to Excel
Name [Units] - <Tag>
Case 1
Case 2
Case 3
Case 4
Case 5
Case 6
Case 7
Case 8
Benzene - Molar Flow [kgmole/h]
0.0000
0.2000
0.4000
0.6000
0.8000
1.000
1.200
1.400
Out - Phase Temperature (Mixed Liquid Phas...
110.3
107.4
104.5
101.5
98.44
95.35
92.24
89.13
Out - Phase Comp Mole Frac (Liquid Phase-B...
0.0000
0.0644
0.1349
0.2125
0.2980
0.3921
0.4954
0.6083
Out - Phase Comp Mole Frac (Vapour Phase-...
0.0000
0.1351
0.2632
0.3840
0.4972
0.6025
0.6993
0.7875
Properties
Simulation
Safety Analysis
Energy Analysis
Messages
Optional Info : Benzene -- Unknown Flow Rate
Optional Info : Benzene -- Not Solved
Optional Info : Toluene -- Unknown Flow Rate
Optional Info : Toluene -- Not Solved
Completed.
Saving case C:\Users\SOUMOD~1\AppData\Local\Temp\AutoRecovery save of NoName (0x88050a).ahc...
Completed.
Solver (Main) - Ready
View Convergence
Responsiveness: 5
100%