SimuTech Project

Simutech Project report on

Process Simulation and modelling in Aspen Plus

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Objective:

To learn general flowsheet simulation concepts ,process design and modelling in Aspen Plus. And to get an understanding of the basic features of Aspen Plus

Acknowledgements

I sincerely express my gratitude to Mentor Nishesh Jyoti for providing me this opportunity to do this project and for his valuable support and advice in making this project possible.

I would also like to thank Shubh Maheshwari and Debanjan Dutta, the head of SimuTech, Chemineers Society and Ashish Kumar President, Chemineers Society who gave me this opportunity to be a part of this project.

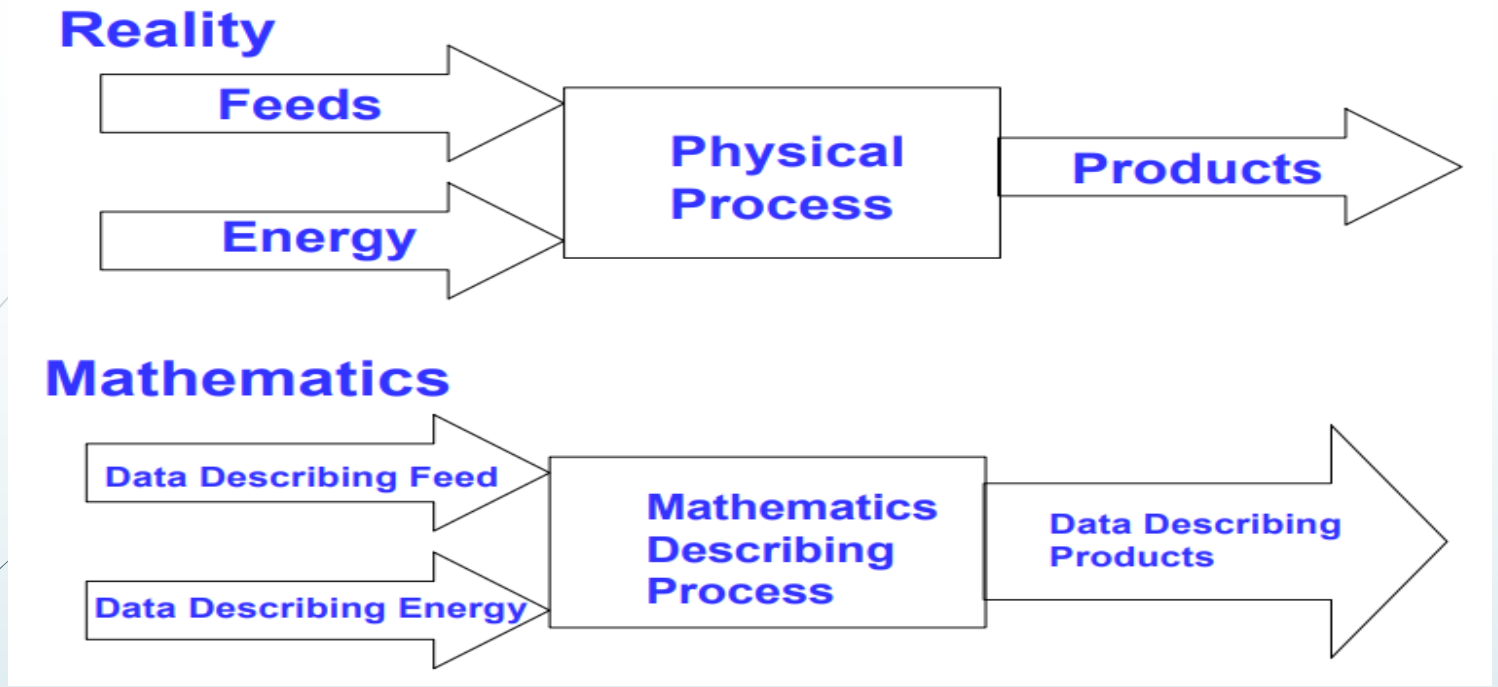
Introduction & Basic Overview

Aspen Plus is a process modeling software that is used widely by the chemical industries for process optimization, process monitoring and process design. It allows the user to design the process and simulate it .

Aspen Plus is a menu driven software which helps us to -

- Predict flow rates, composition, physical properties of process streams.
- Predict operating conditions for the processes, pre sizing of equipments, and how to connect the equipments(menu driven equipments) .
- Aspen plus itself codes the physical relations associated with these menu driven equipments in the background and will have unique equations called characteristic equations(i.e. mass balances, energy balances , rate equations, vapour liquid equilibrium)
- It takes a design that the user supplies and simulates the performance of the process specified in that design.

Process Simulation



Unit Operation Model Types

- Mixers/Splitters - Mixer, FSplit, SSplit

- Separators - Flash2, Flash3, Decanter, Sep
- Heat Exchangers – Heater, HeatX

- Columns – DSTWU, Distl, RadFrac

- Reactors – RYeild, RStoic, REquil, RGibbs, RCSTR, RPlug, RBatch.

Steps for developing a simulation:

- Defining the components (like water, ethanol, benzene etc.) Specifying what chemical components will be present in the streams of the flowsheet. Components can be searched by using the Find button. We can find various components using their molecular weight, or boiling points etc.
- Specification of Thermodynamic Methods(property method, process type).
- Select the units of measurement for input data and output.
- Developing the process flow diagram (Mainstream), which consists of the unit operations (blocks) and streams that feed and connect the blocks(mixer, separators, exchangers, columns, reactors, etc.) Convert the process flowsheet into unit operating blocks and choose an appropriate model for each block.
- Adding desired streams to the block (material / energy)which shows arrows where the stream can be connected. Red arrows indicate required streams and blue arrows indicate optional streams.
- Addition of various components to various streams.
- Entering compound information
- Entering information at locations where there are red semicircles, that means required inputs are incomplete.
- Specifying Stream and Block Information that is -the stream composition(mole fractions, mass fractions, mass flow rates or molar low rates etc.), total feed flow rate, and state for feed streams (pressure, temperature, vapour fraction etc.)
- Running the simulation and Viewing Results.

Mixer –

Stream mixing , adding heat streams, adding work streams. Combine multiple streams into one stream.

FSplit-

Split stream flows, Stream splitter.
We need to specify feed input conditions(Temperature, pressure, total flow rate with units, different component composition), split fractions.

SSplit-

Substream splitter, Split substream flows.
We need to specify split fraction of outlet streams.

Flash2- Single stage distillation column

Two-outlet flash, determine thermal and phase conditions, separates vapour and liquid at VLE. Temperature and pressure of flash is kept in between the boiling points of the two components. We get the lighter component from the top stream and heavier at the bottom. To get the heavier component from the top we select that component as key component.

Flash3-

Three-outlet flash

Decanter-

Liquid-liquid decanter, single stage separators with two liquid phases and no vapor phase.

Sep-

Multi-outlet component separator, separate inlet stream components into any number of outlet streams. We need to specify split fraction of outlet streams.

Heater-

Heater or cooler. When using single heater , for heater we need to specify either temperature or pressure and heat duty.
If we are exchanging heat between two heaters then we require only temperature or pressure for the second heater.

HeatX- Need to specify two hot and cold streams.
Two-stream heat exchanger, exchange heat between two streams.

Shortcut method- Performs simple material and energy balance calculations, and is used where geometry is unknown or unimportant.

Shell and tube Method

-Rating shell and tube heat exchangers when geometry is known- Rating is done to know whether the tube is overdesigned or under designed.

-In exchanger details in thermal results actual exchanger area should be close to required exchanger area. To adjust the area we can alter tube length or number of tubes

DSTWU- Shortcut distillation design

Determine minimum RR, minimum stages, and either actual RR or actual stages by Winn-Underwood Gilliland method

Columns with one feed and two product streams.

Reflux ratio= 1.3 times of Rminimum which is written as -1.3

RadFrac- Rigorous fractionation

Rigorous rating and design for single columns. Outputs of DSTWU are used in its inputs (like Distillate to feed ratio, number of actual stages, feed stage, actual reflux ratio)

Specify Condenser type, phases, reboiler type, tray type, starting and ending stage etc.

Distl-

Shortcut distillation rating. Determine separation based on RR, stages, and D:F ratio.
Columns with one feed and two product streams. Outputs of DSTWU are used in its inputs (like Distillate to feed ratio, number of actual stages, feed stage, actual reflux ratio)
Need to specify condenser and reboiler pressure.

Reactors –

Balance based-

-RYeild- Only mass balance, no atom balancing. Used to simulate reactors in which inlets to the reactor are not completely known but outlets are known (e.g., to simulate a furnace).

-RStoic- Requires both an atom and a mass balance. Used where both the equilibrium data and the kinetics are either unknown or unimportant.

Equilibrium based-

Do not take reaction kinetics into account.

-REquil-

Computes combined chemical and phase equilibrium by solving reaction equilibrium equations.
Useful when there are many components, a few known reactions, and when relatively few components take part in the reactions.

-RGibbs-

Useful when reactions occurring are not known or are high in number due to many components participating in the reactions.

This is the only Aspen Plus block that will deal with solid-liquid gas phase equilibrium.

Kinetics based-

Reaction kinetics are taken into account.

-RCSTR-

Used when reaction kinetics are known and when the reactor contents have same properties as outlet stream.

Allows for any number of feeds, which are mixed internally.

Up to three product streams are allowed - vapor, liquid1, liquid2 or vapor, liquid, free water.

-RPlug-

Handles only rate-based reactions.

A cooling stream is allowed.

We must provide reactor length and diameter.

-RBatch-

Handles rate-based kinetics reactions only.

Any number of continuous or delayed feeds are allowed .

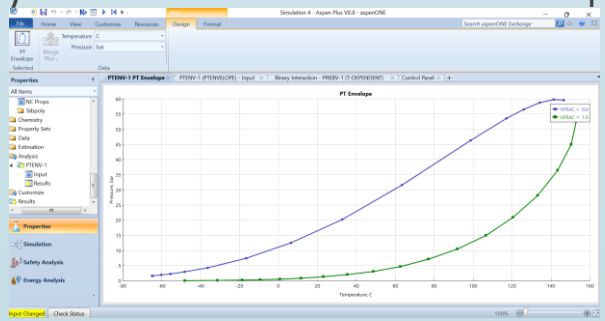
Must provide one of the following: stop criteria, cycle time, or result time.

Drawing various curves in aspen

1)Pure analysis- Using this we can get the curve of any property of the component (cp, cv, density) over a temperature range or discrete temperature values.

2) PT envelope-To show the phases of a substance. Line separating solid and vapor phases is sublimation line. Line separating solid and liquid phases is fusion line. Line separating liquid and vapor phases is vaporization line. The point where three lines meet is called the triple point where all three phases can exist in equilibrium. The point where vaporization line ends is called the critical point. At temperatures and pressures greater than those at the critical point, no substance can exist as liquid no matter how great pressure is exerted upon it.

PT envelope (for pure component)- It gives the curve of pressure vs temperature for a particular flow rate of any component.
we can compare the properties of different component by merging their plots.
PT envelope (for binary system)-Using this we get the of pressure vs temperature curve at particular flow rates of two components (in a fixed ratio). Between the curves vapour and liquid will be in equilibrium (as seen in the figure)



3) Binary Analysis

Using this we can plot T-xy , P-xy, Gibbs energy and y vs x plot for binary systems (VLE) , where x and y are the liquid and vapour mole fractions of any one component and that are in equilibrium. Between the curves VLE exists.
Tie line- A constant temperature line representing mole fraction of a component in liquid and vapour phase (also shown in the figure below).
T- xy graph is plotted at constant pressure and P- xy is plotted at constant temperature.

Assignment 1

Problem statement-Practice each (same) problem covered in session 2b, 3 & 4, which covers

1). Pure (property graph and merging of graphs for property comparison) and Binary analysis (Txy, Pxy & xy diagram)

2). Mixer/Splitters (Mixer, FSplit, SSplit)

3). Separators (Flash2, Flash3, Decanter, Sep)

4). Exchangers (Heater, HeatX)

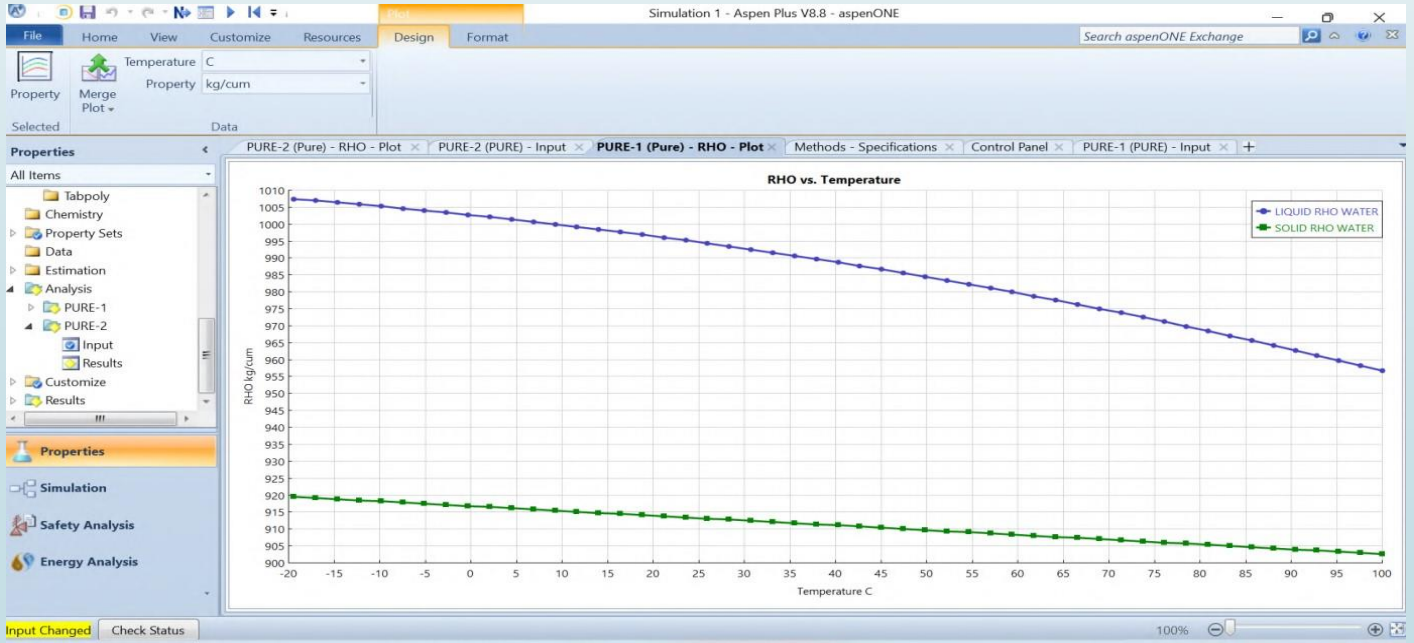
5). Columns (DSTWU, Distl, RadFrac) Hint: Use output of DSTWU as input for Distl & RadFrac column.

Solution:

1)

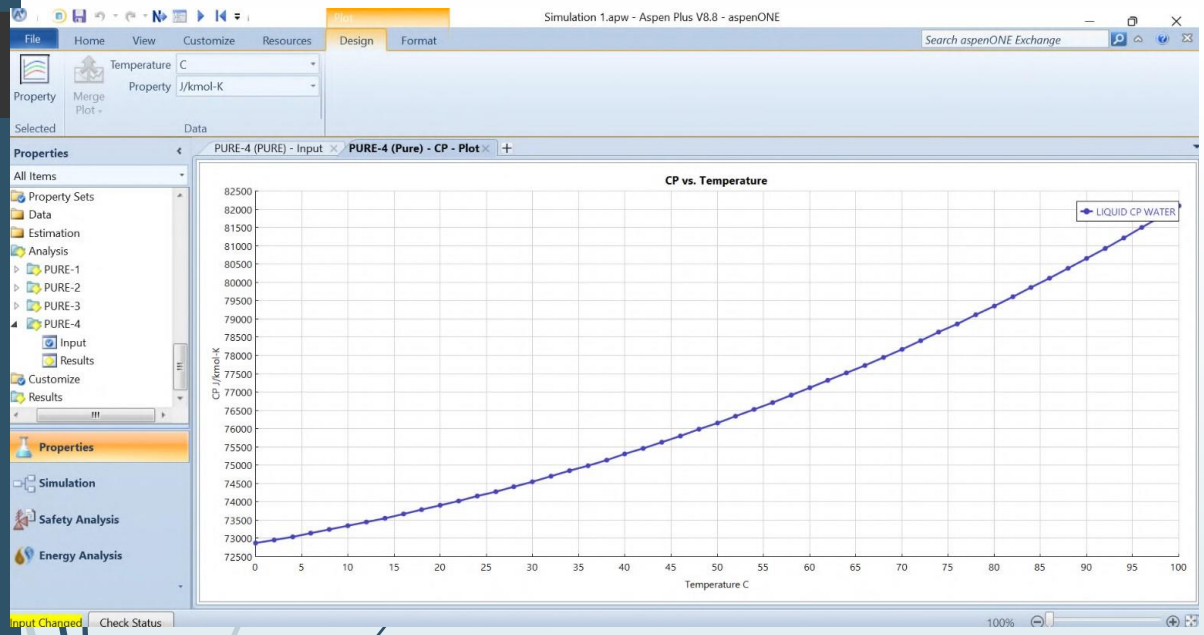
a) For pure water – Density vs Temperature for vapour and liquid phase (for a temperature range of -19.42 to 100 degree celcius)

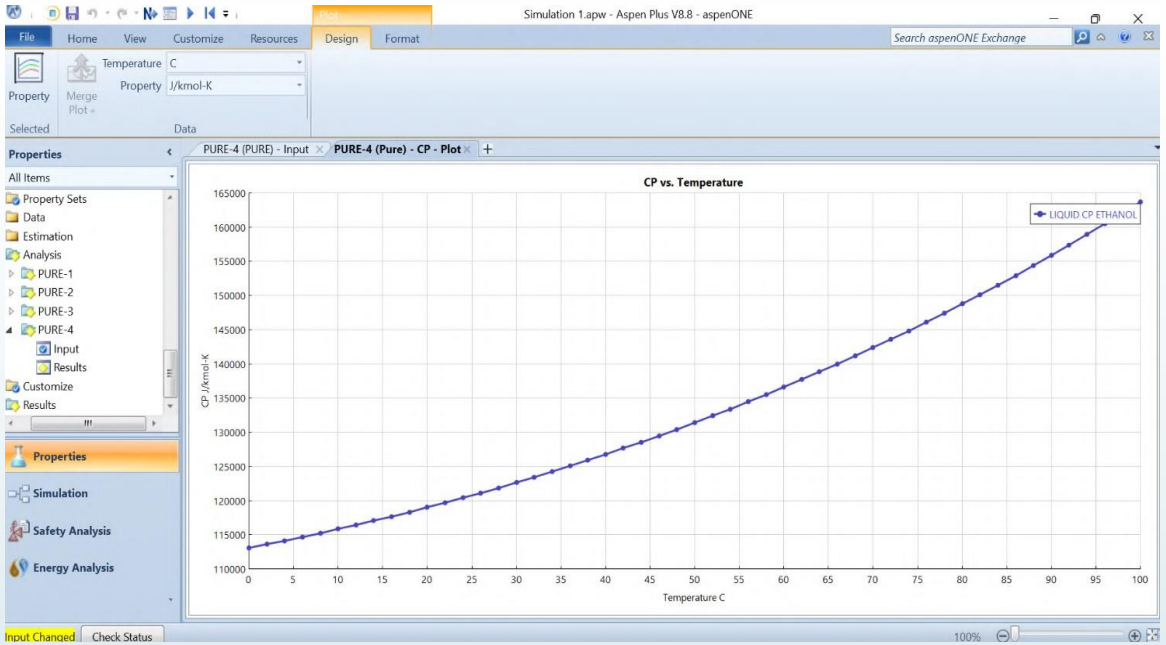
Pressure=1.59325 Bar, Property Method-NRTL



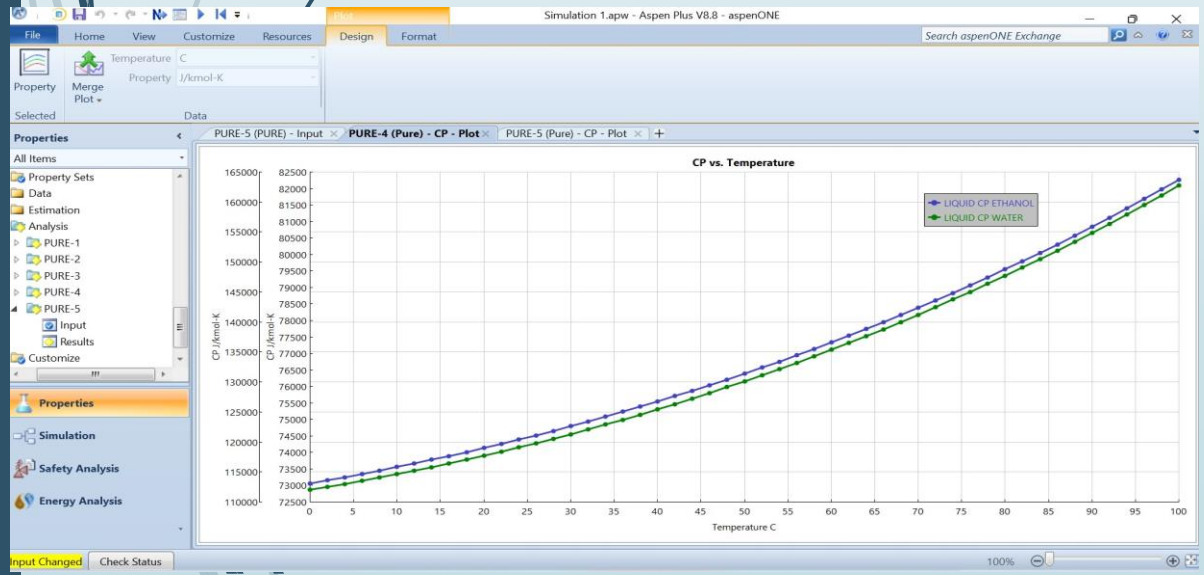
CP vs temperature of water and ethanol binary system, Property method-NRTL

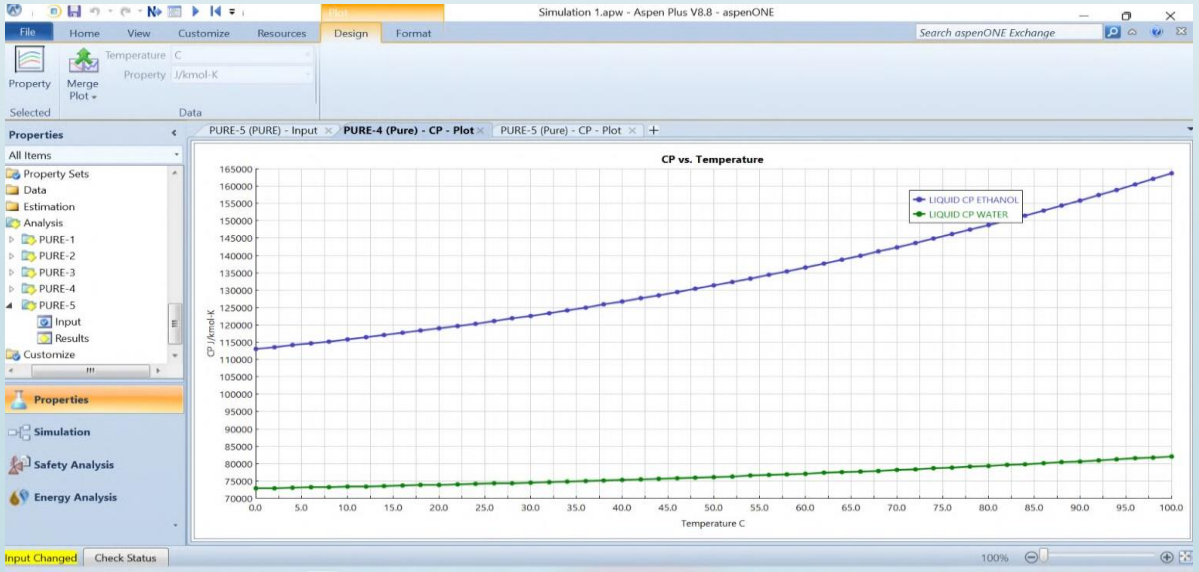
Individual plots-





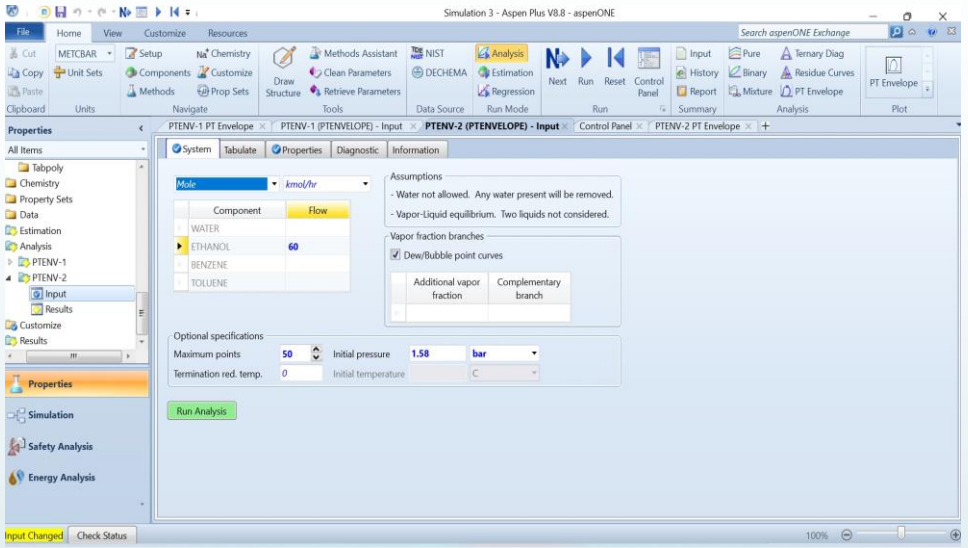
Merged curves

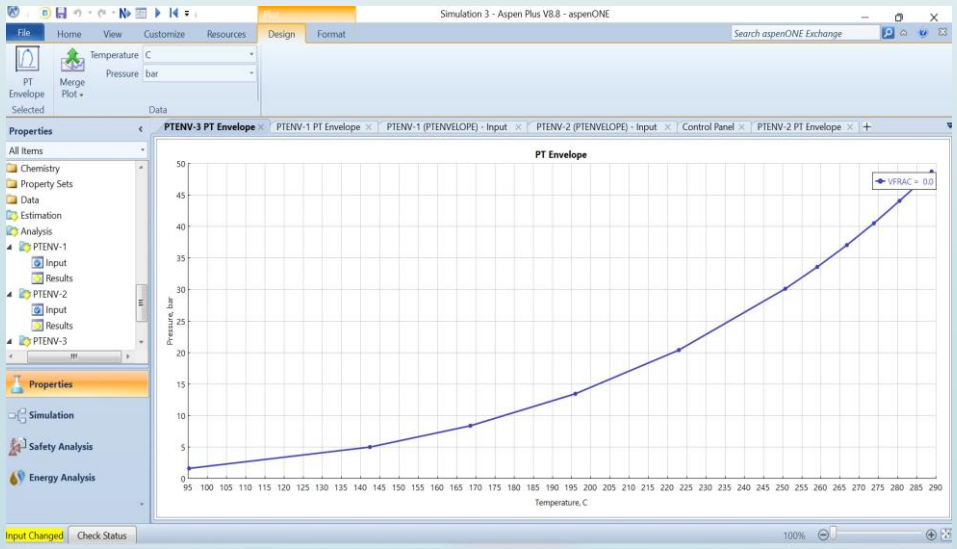


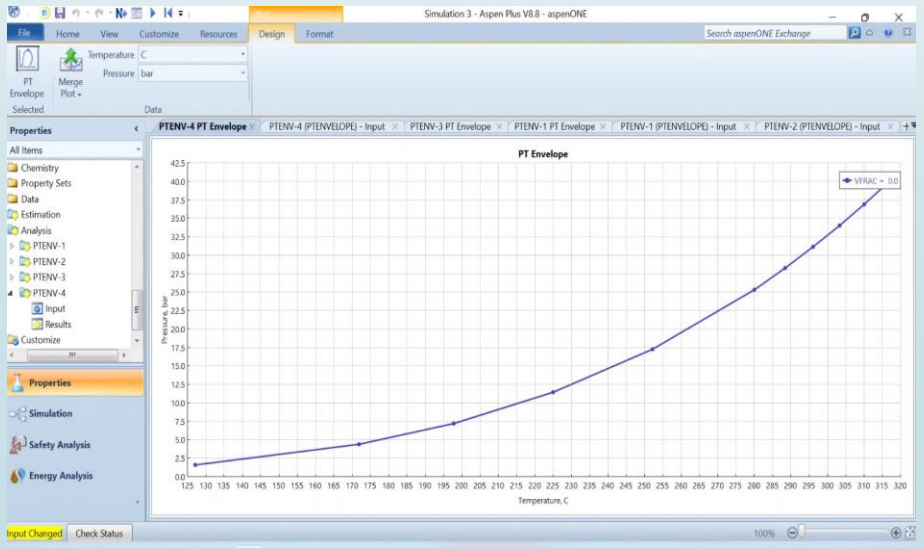


PT envelopes of pure components and their comparison (water, ethanol, benzene, toluene-in order)

Pressure=1.58 Bar, Molar flow rate of each component=60 Kmol/hr

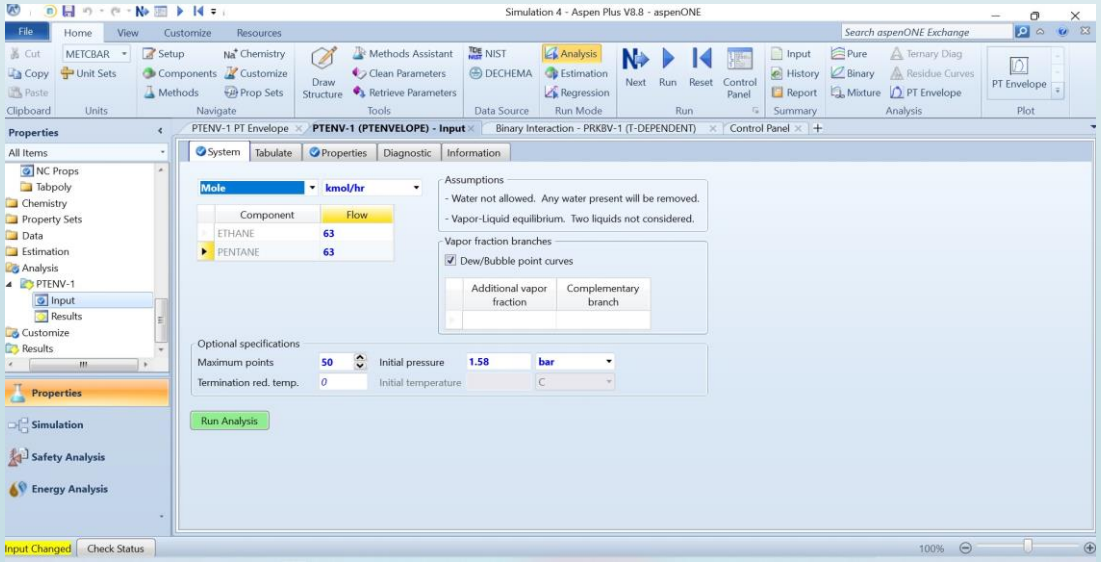




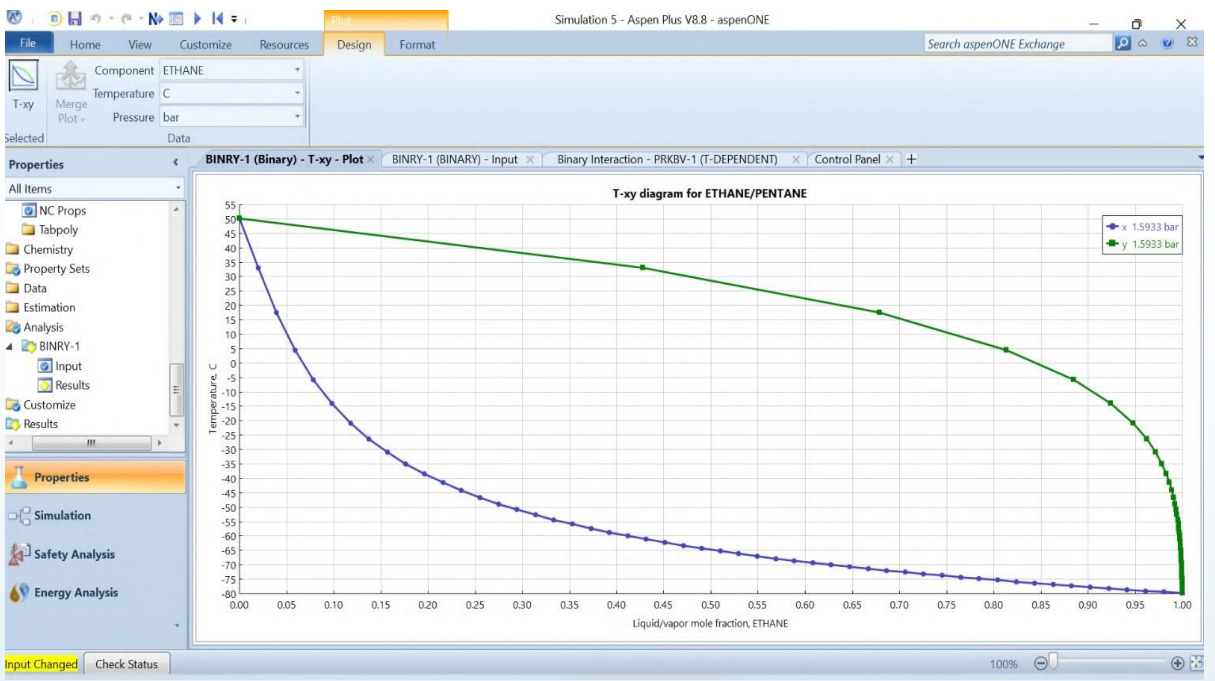


Merged curves

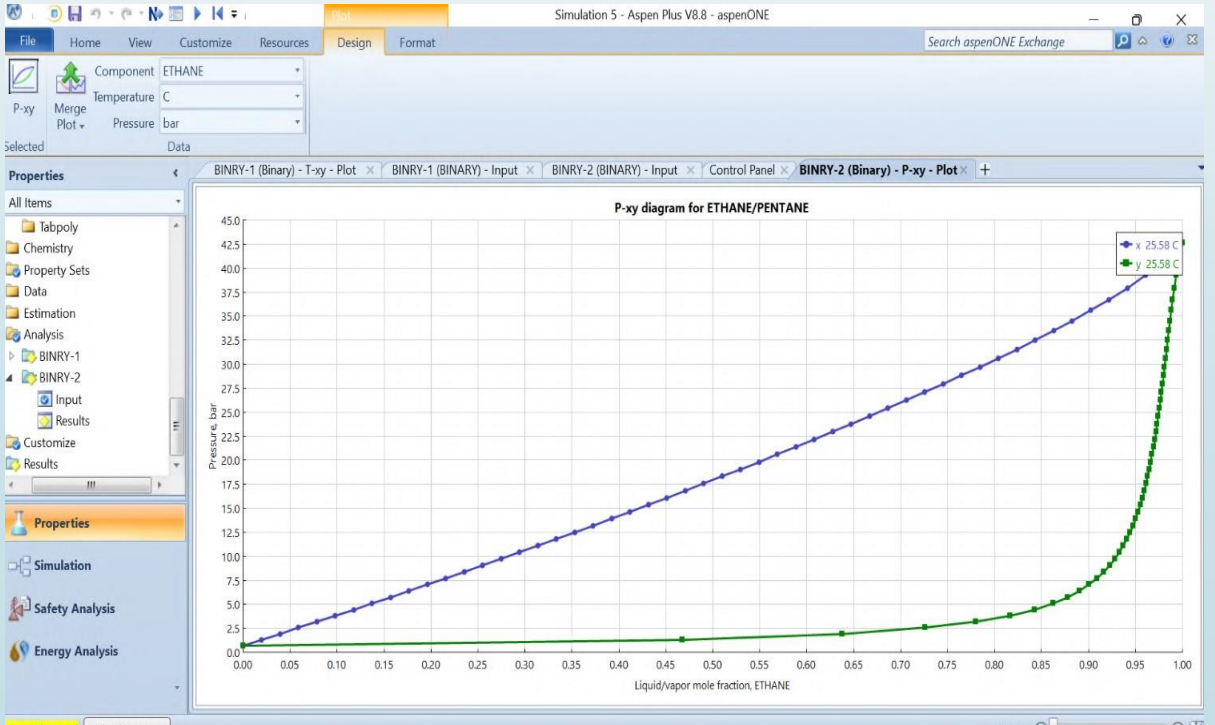
For binary system of ethane and pentane -PT envelope



T- xy plot – For ethane and pentane (Mole basis)
Pressure=1.59325 Bar
Property Method= PENG-ROB



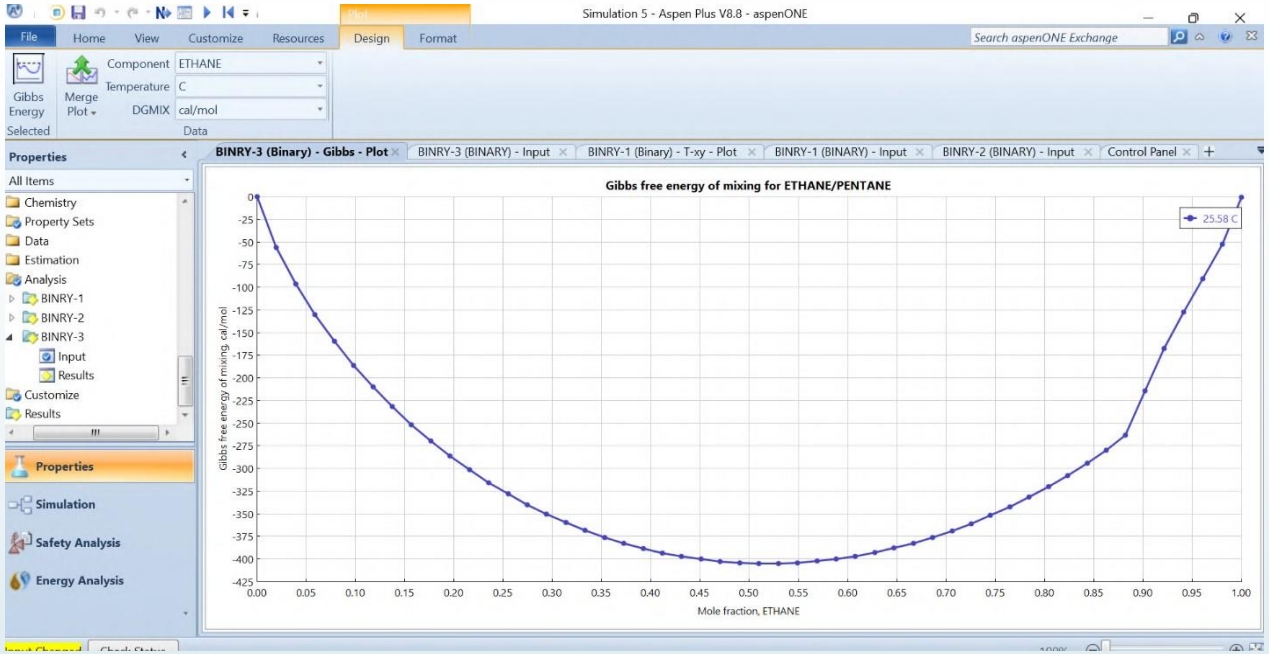
P -xy plot For ethane and pentane (Mole basis)
Temperature=25.58 degree celcius
Property Method= PENG-ROB



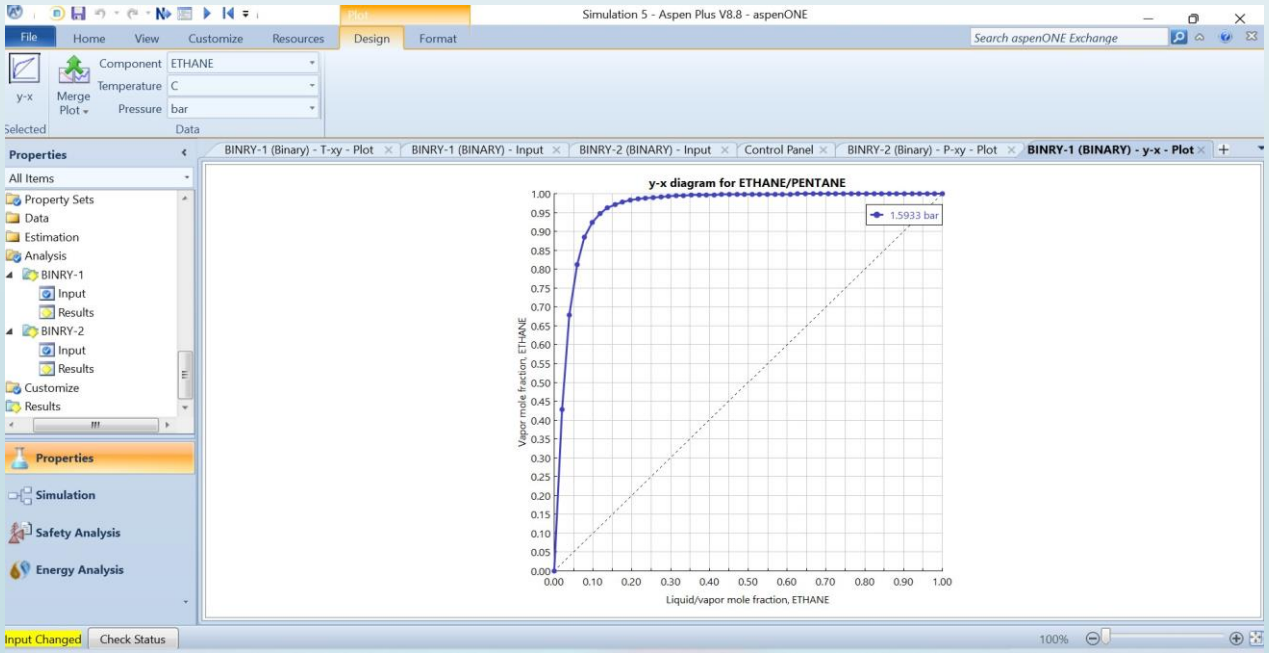
Gibbs energy plot-For ethane and pentane (Mole basis)

Pressure=1.59325 Bar, Temperature=25.58 degree celcius

Property Method= PENG-ROB



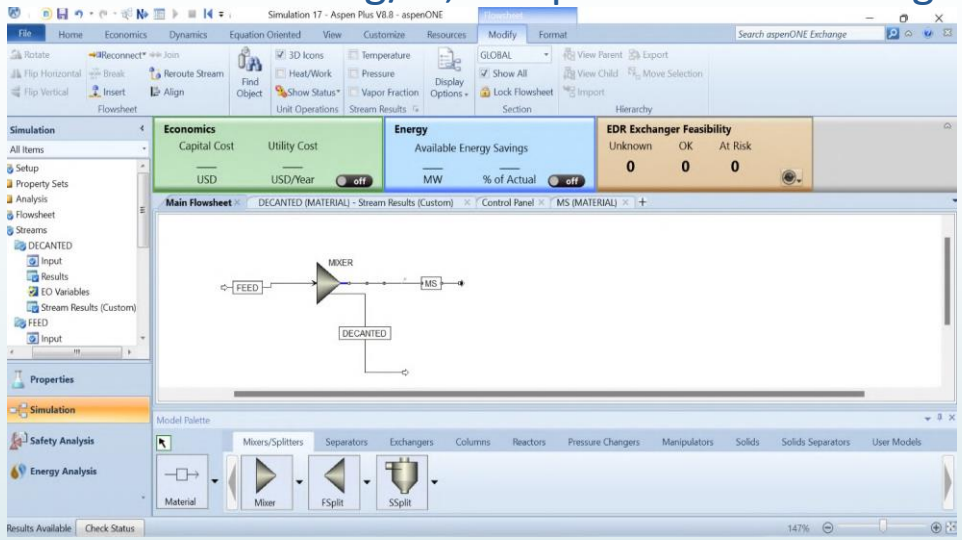
Y vs X



2). Mixer/Splitters (Mixer, FSplit, SSplit) with decanted stream

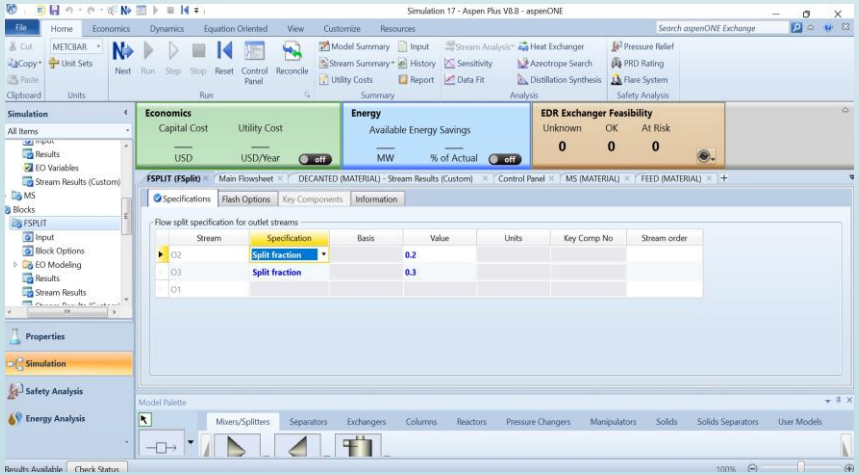
Mixer -Feed -Benzene, water, toluene, mass fractions=0.3, 0.2, 0.5 respectively.

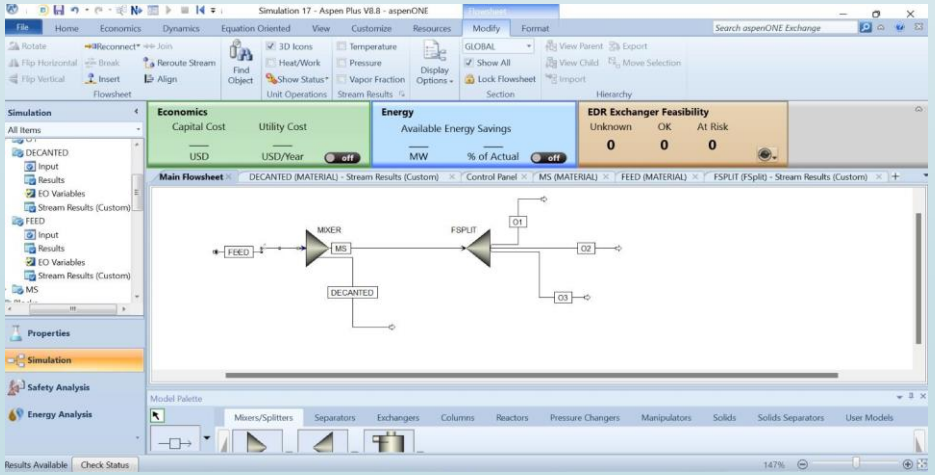
Total Mass flow rate=3000kg/hr, Temperature=25.58 degree celcius, pressure=1.58 atm



Fsplit-Feed -Benzene, water, toluene, mass fractions=0.3, 0.2, 0.5 respectively.

Total Mass floe rate=3000kg/hr, Temperature=25.58 degree celcius, pressure=1.58 atm

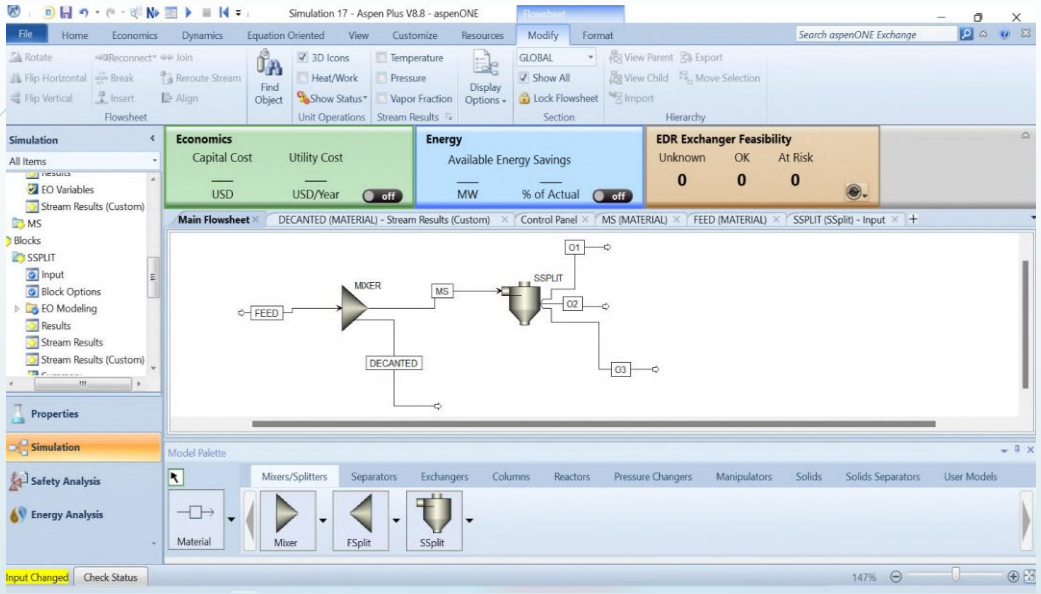




From To Substream: MIXED Phase: Component Mole Flow	Units	Stream Results MS MIXER FSPLIT Liquid	 O1 FSPLIT Liquid	O2 FSPLIT Liquid Page 1/2 2022-05-21 11:49:30
BENZENE	KMOL/HR	11.74443	5.872214	2.348886
WATER	KMOL/HR	0.1302309	0.0651154	0.0260461
TOLUENE	KMOL/HR	16.59422	8.29711	3.318844
Mole Flow	KMOL/HR	28.46888	14.23444	5.693776
Mass Flow	KG/HR	2448.746	1224.373	489.7492
Volume Flow	L/MIN	47.88151	23.94075	9.576302
Temperature	C	39.67601	39.67601	39.67601
Pressure	BAR	1.600935	1.600935	1.600935
Vapor Fraction		0	0	0
Liquid Fraction		1	1	1
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	6716.411	6716.411	6716.411
Mass Enthalpy	CAL/GM	78.08432	78.08432	78.08432
Enthalpy Flow	CAL/SEC	53113.52	26556.76	10622.7
Molar Entropy	CAL/MOL-K	-69.69254	-69.69254	-69.69254
Mass Entropy	CAL/GM-K	-0.8102385	-0.8102385	-0.8102385
Molar Density	MOL/CC	0.00990949	0.00990949	0.00990949
Mass Density	GM/CC	0.8523632	0.8523632	0.8523632
Average Molecular Weight		86.01485	86.01485	86.01485

From To Substream: MIXED	Units	Stream Results O3 FSPLIT Liquid	 DECANTED MIXER Liquid	FEED MIXER Liquid
BENZENE	KMOL/HR	3.523328	0	11.74443
WATER	KMOL/HR	0.0390692	33.81873	33.94896
TOLUENE	KMOL/HR	4.978266	0	16.59422
Mole Flow	KMOL/HR	8.540663	33.81873	62.28761
Mass Flow	KG/HR	734.6238	609.2539	3058
Volume Flow	L/MIN	14.36445	10.23149	54.84273
Temperature	C	39.67601	39.67601	25.58
Pressure	BAR	1.600935	1.600935	1.600935
Vapor Fraction		0	0	0
Liquid Fraction		1	1	1
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	6716.411	-68004.83	-33853.09
Mass Enthalpy	CAL/GM	78.08432	-3774.841	-689.5448
Enthalpy Flow	CAL/SEC	15934.06	-638840	-585730
Molar Entropy	CAL/MOL-K	-69.69254	-38.12094	-53.80933
Mass Entropy	CAL/GM-K	-0.8102385	-2.116034	-1.096028
Molar Density	MOL/CC	0.00990949	0.0550892	0.0189291
Mass Density	GM/CC	0.8523632	0.9924488	0.929324
Average Molecular Weight		86.01485	18.01528	49.09484

Ssplit- Feed and conditions are same as FSplit



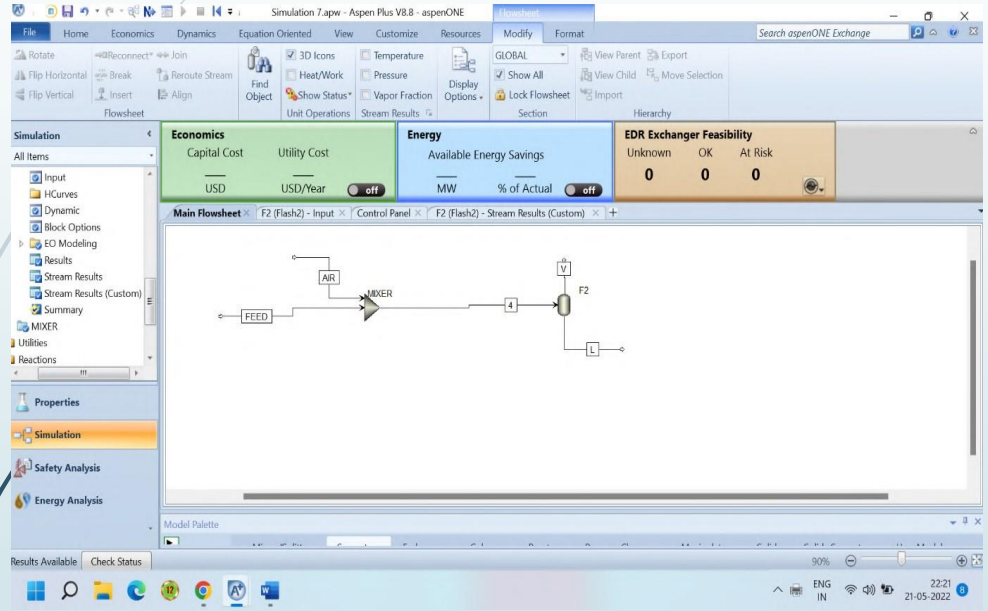
Volume Flow	L/MIN	23.94075
Temperature	C	39.67601
Pressure	BAR	1.600935
Vapor Fraction		0
Liquid Fraction		1
Solid Fraction		0
Molar Enthalpy	CAL/MOL	6716.411
Mass Enthalpy	CAL/GM	78.08432
Enthalpy Flow	CAL/SEC	26556.76
Molar Entropy	CAL/MOL-K	-69.69254
Mass Entropy	CAL/GM-K	-0.8102385
Molar Density	MOL/CC	0.009909 49
Mass Density	GM/CC	0.852363 2
Average Molecular Weight		86.01485

3). Separators (Flash2, Flash3, Decanter, Sep) Method-NRTL

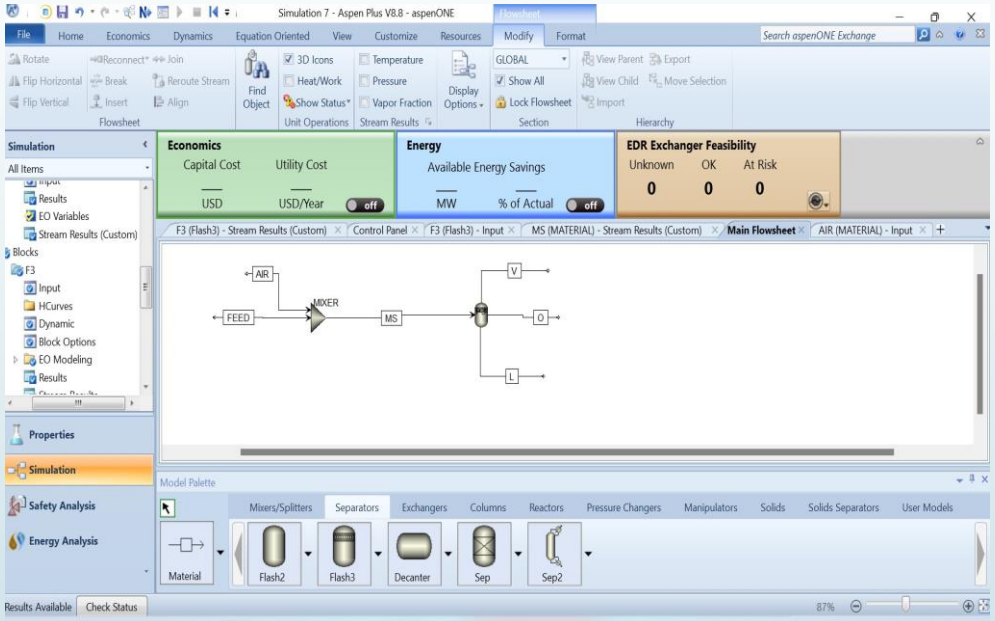
MIXER AND FLASH (INPUT- Naphthalene, Toluene, Water with 0.18, 0.26, 0.56 mole fractions respectively and Temp=25.58 degree celcius, pressure=2.08 atm, Total flow rate=1058 kg/h

AIR-Temp=25.58 deg celcius, Pressure=2.04 atm , Flow rate=558 kg/h

Flash- Temp.=50.58 deg celcius, Pressure= 1.78 Bar



Flash2



Flash3

Stream Results				
	Units	4	L	V
From		MIXER	F2	F2
To		F2		
Substream: MIXED Phase:				
Component Mole Flow		Mixed	Liquid	Vapor
NAPHT-01	KMOL/HR	3.334248	3.32458	0.00966815
TOLUENE	KMOL/HR	4.816136	2.756811	2.059325
WATER	KMOL/HR	10.37322	8.162075	2.211141
AIR	KMOL/HR	19.27401	0.0132408	19.26077
Mole Flow	KMOL/HR	37.79761	14.25671	23.5409
Mass Flow	KG/HR	1616	827.5625	788.4375
Volume Flow	L/MIN	3817.622	14.02154	
Temperature	C	17.17647	50.58	5855.249
Pressure	BAR	2.10756	1.803585	50.58
Vapor Fraction		0.5267614	0	1.803585
Liquid Fraction		0.4732386	1	1
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	-16258.03	-32341.64	0
Mass Enthalpy	CAL/GM	-380.2689	-557.1606	-4138.758
Enthalpy Flow	CAL/SEC	-170700	-128080	-123.5736
				-27063.91
Molar Entropy	CAL/MOL-K	-29.26044	-55.64179	-5.298683
Mass Entropy	CAL/GM-K	-0.6843902	-0.9585605	-0.1582063
Molar Density	MOL/CC	0.000165014	0.0169462	6.7008E-05
Mass Density	GM/CC	0.007055	0.9836799	0.00224425
Average Molecular Weight		42.75403	58.04724	33.49224

Flash2

Stream Results				
	Units	L	MS	O
From		F3	MIXER	F3
To			F3	
Substream: MIXED Phase:				
Component Mole Flow		Liquid	Mixed	Liquid
WATER	KMOL/HR	8.769641	10.37322	0.0583612
TOLUENE	KMOL/HR	0.000855648	4.816136	3.987374
NAPHT-01	KMOL/HR	6.57192E-05	3.334248	3.323174
AIR	KMOL/HR	0.000954181	19.27401	0.0148881
Mole Flow	KMOL/HR	8.771517	37.79761	7.383797
Mass Flow	KG/HR	158.1024	1616	794.824
Volume Flow	L/MIN	2.719845	3866.975	14.33603
Temperature	C	50.58	17.03054	50.58
Pressure	BAR	1.78	2.08	1.78
Vapor Fraction		0	0.5268889	0
Liquid Fraction		1	0.4731111	1
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	-67787.18	-16264.84	12578.28
Mass Enthalpy	CAL/GM	-3760.83	-380.4283	116.8504
Enthalpy Flow	CAL/SEC	-165170	-170770	25798.75
Molar Entropy	CAL/MOL-K	-37.49129	-29.26657	-78.17417
Mass Entropy	CAL/GM-K	-2.080015	-0.6845337	-0.7262264
Molar Density	MOL/CC	0.0537501	0.000162908	0.0085842
Mass Density	GM/CC	0.9688201	0.00696496	0.9240402
Average Molecular Weight		18.02453	42.75403	107.6443

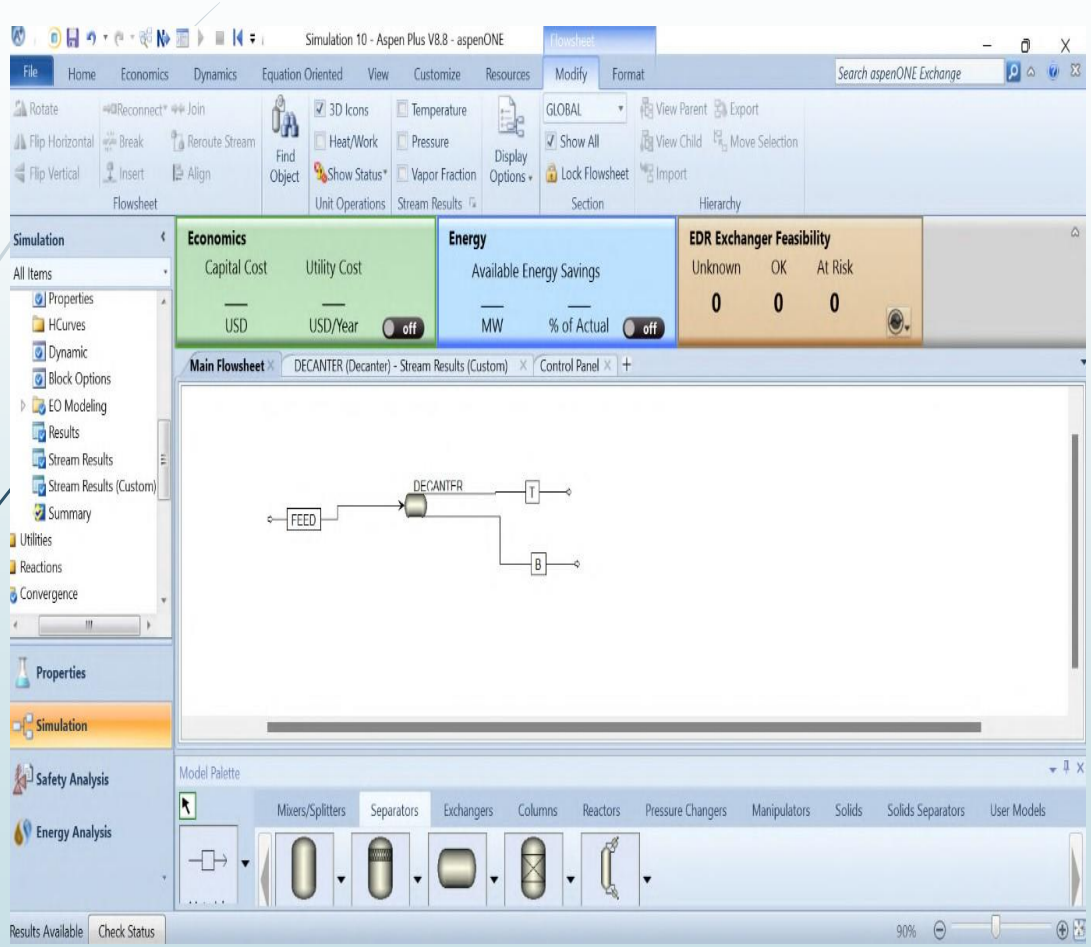
From			
To			
Substream: MIXED			
Phase:			
Component Mole Flow	Units KMOL/HR	V	
WATER		F3	
TOLUENE			
NAPHT-01		Vapor	
	KMOL/HR	1.545214	
	KMOL/HR	0.8279064	
	KMOL/HR	0.0110087	

Flash3

AIR	KMOL/HR	19.25816
Mole Flow	KMOL/HR	21.64229
Mass Flow	KG/HR	663.0736
Volume Flow	L/MIN	5454.34
Temperature	C	50.58
Pressure	BAR	1.78
Vapor Fraction		1
Liquid Fraction		0
Solid Fraction		0
Molar Enthalpy	CAL/MOL	-3448.636
Mass Enthalpy	CAL/GM	-112.5613
Enthalpy Flow	CAL/SEC	-20732.33
Molar Entropy	CAL/MOL-K	-2.639369
Mass Entropy	CAL/GM-K	-0.0861473
Molar Density	MOL/CC	6.61317E-05
Mass Density	GM/CC	0.00202613
Average Molecular Weight		30.63786

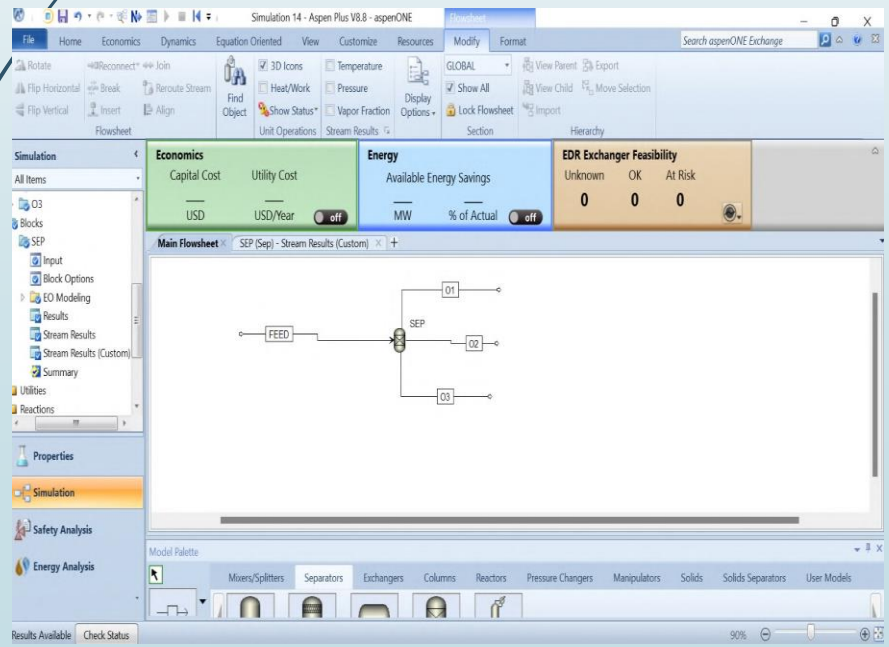
AIR

DECANTER (P- xylene and water-Temp=30.58 deg celcius, Pressure=1.58 atm, Total flow rate=2058kg/h, and 0.5 mass fraction of both components)
Decanter- Temp=40.58 deg celcius,, Pressure=1.58 Bar



From To Substream: MIXED	Stream Results Units	B DECANTER	FEED DECANTER	T DECANTER
Phase:		Liquid	Liquid	Liquid
Component Mole Flow				
P-XYL-01	KMOL/HR	0.00228087	9.692241	9.689959
WATER	KMOL/HR	57.09191	57.11818	0.0262699
Mole Flow	KMOL/HR	57.09419	66.81042	9.716229
Mass Flow	KG/HR	1028.769	2058	1029.231
Volume Flow	L/MIN	17.51816	36.69788	20.22996
Temperature	C	40.58	30.58	40.58
Pressure	BAR	1.58	1.600935	1.58
Vapor Fraction		0	0	0
Liquid Fraction		1	1	1
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	-67981.36	-59046.05	-5295.488
Mass Enthalpy	CAL/GM	-3772.802	-1916.857	-49.99089
Enthalpy Flow	CAL/SEC	-1078200	-1095800	-14292.27
Molar Entropy	CAL/MOL-K	-38.06154	-49.38345	-105.4639
Mass Entropy	CAL/GM-K	-2.112323	-1.603173	-0.9956085
Molar Density	MOL/CC	0.054319	0.0303425	0.00800482
Mass Density	GM/CC	0.9787644	0.9346589	0.8479429
Average Molecular Weight		18.0188	30.80358	105.9291

SEPARATOR – RK-ASPEN Method
(Input- benzene and water,
Temp=120.58 deg celcius,
Pressure=1.58 atm, Total flow rate=158 kmol/h with 0.6 and 0.4 mol fractions of components respectively)
Output streams-1st stream=0.7 split fraction of benzene(water free), 2nd stream=0.7 split fraction of water(benzene free), 3rd stream=0.3 split fraction for both water and benzene



Stream Results				
From	Units	FEED	O1 SEP	O2 SEP
To		SEP		
Substream: MIXED Phase:				
Component Mole Flow BENZENE		Vapor	Vapor	Vapor
WATER				
Mole Flow	KMOL/HR	94.8	66.36	28.44
Mass Flow	KMOL/HR	63.2	0	18.96
Volume Flow	KMOL/HR	158	66.36	47.4
Temperature	KG/HR	3543.739	3183.621	2563.122
Pressure	L/MIN	52610.17	21861.29	15783.05
Vapor Fraction	C	120.58	120.58	120.58
Liquid Fraction	BAR	1.600935	1.600935	1.600935
Solid Fraction		1	1	1
Molar Enthalpy		0	0	0
Mass Enthalpy		0	0	0
Enthalpy Flow		0	0	0
Molar Entropy	CAL/MOL	-9637.867	21937.71	-57009.65
Mass Entropy	CAL/GM	-178.2338	280.8435	-3164.516
Molar Density	CAL/SEC	-423000	404385	-700590
Mass Density	CAL/MOL-K	-21.61685	-32.05558	-9.313488
Average Molecular Weight	CAL/GM-K	-0.399762	-0.4103711	-0.5169771
	MOL/CC	5.00537E-05	5.05917E-05	4.94765E-05
	GM/CC	0.00270662	0.0039519	0.000891333
		54.0743	78.11364	18.01528
From				
To				
Substream: MIXED	Units KMOL/HR	O3		
Phase:		SEP		
Component Mole Flow				
BENZENE	KMOL/HR	47.4		
WATER	KMOL/HR	2563.122		
Mole Flow	KG/HR	15783.05		
Mass Flow	L/MIN			
Volume Flow		Vapor		

Temperature	C	120.58
Pressure	BAR	1.600935
Vapor Fraction		1
Liquid Fraction		0
Solid Fraction		0
Molar Enthalpy	CAL/MOL	-9637.867
Mass Enthalpy	CAL/GM	-178.2338
Enthalpy Flow	CAL/SEC	-126900
Molar Entropy	CAL/MOL-K	-21.61685
Mass Entropy	CAL/GM-K	-0.399762
Molar Density	MOL/CC	5.00537E-05
Mass Density	GM/CC	0.00270662
Average Molecular Weight		54.0743

4). Exchangers (Heater, HeatX)

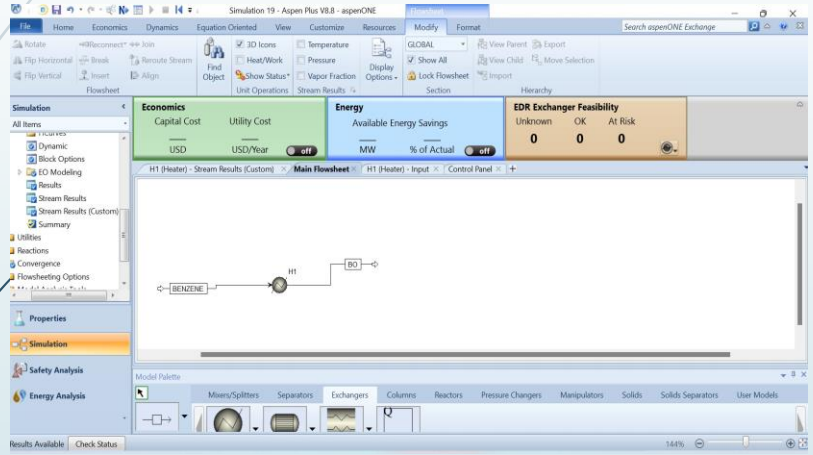
HEATER

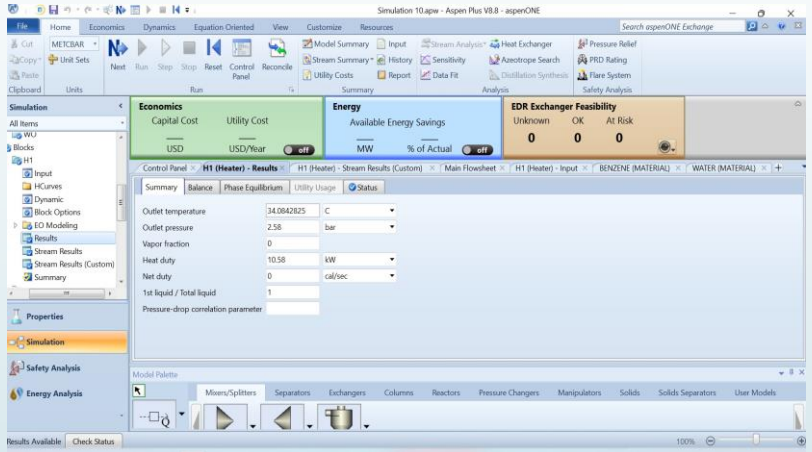
Feed-Water(Temp=300.58 deg celcius, Pressure=10.58 Bar, Flow rate=658 kg/h)

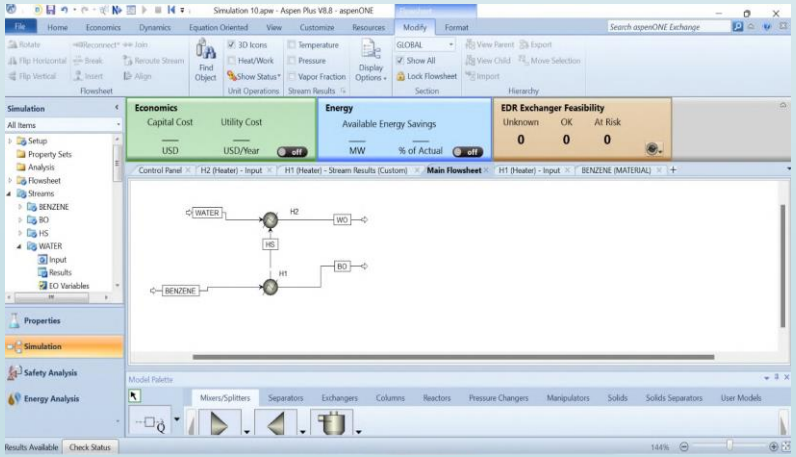
Benzene(Temp=30.58 deg celcius, Pressure=2.58 Bar, Flow rate=6058 kg/h)

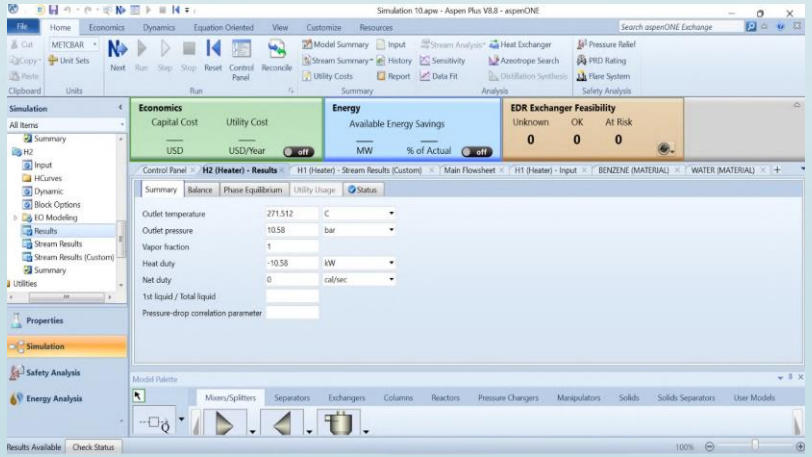
H1(Pressure=2.58 Bar, Heat duty=10.58 KW,

H2(Pressure=10.58 bar









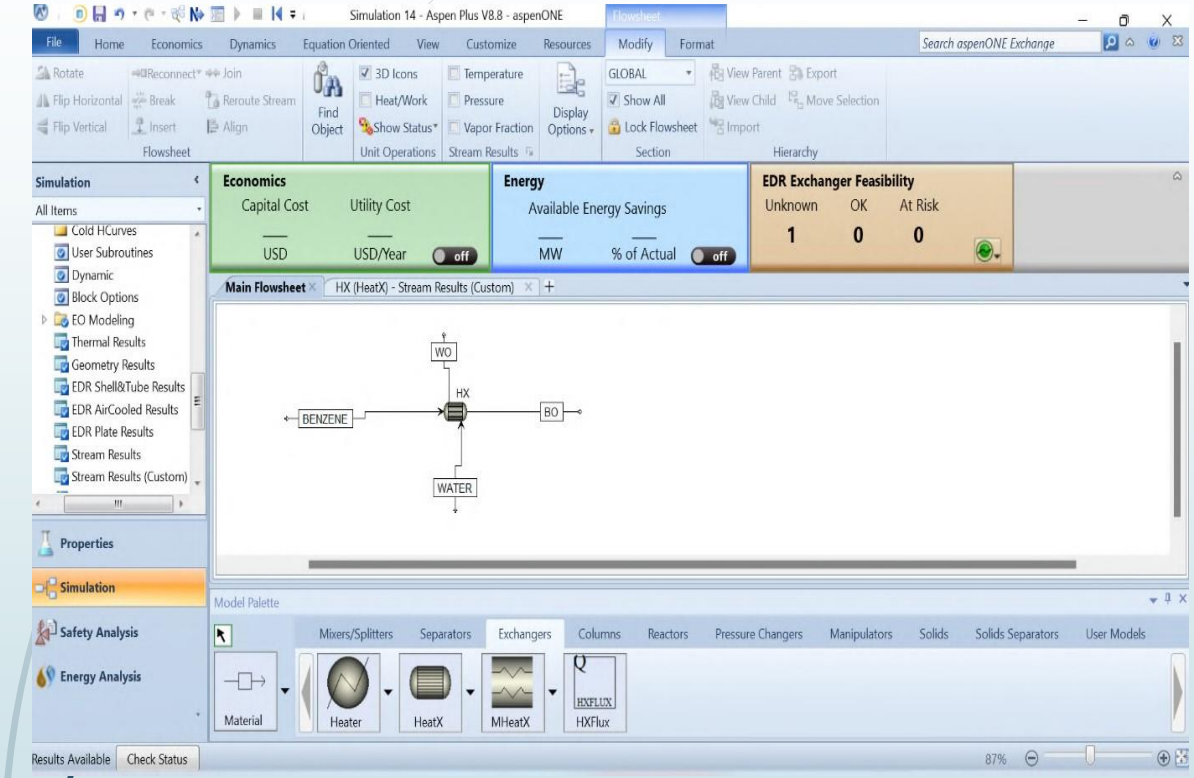
Stream results H1

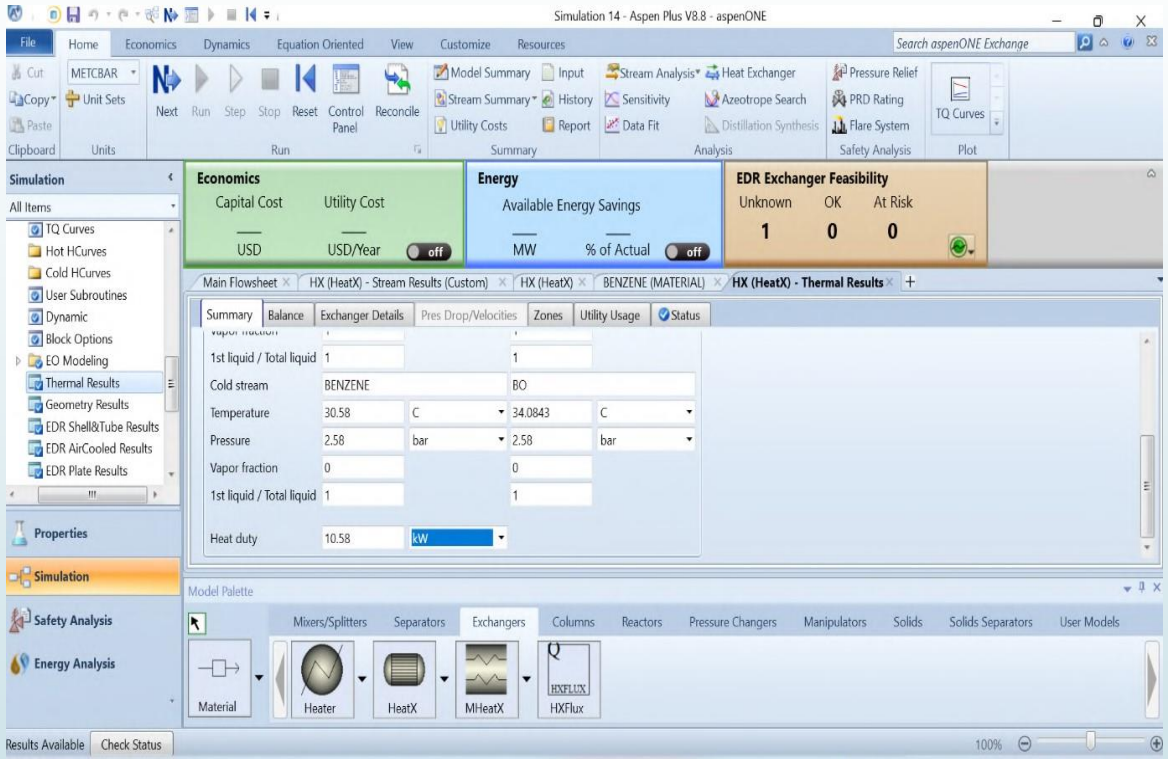
	Units	BENZENE	BO
From			H1
To Substream: MIXED		H1	
Phase: Component Mole Flow		Liquid	Liquid
WATER	KMOL/HR	0	0
BENZENE	KMOL/HR	77.55368	77.55368
Mole Flow	KMOL/HR	77.55368	77.55368
Mass Flow	KG/HR	6058	6058
Volume Flow	L/MIN	116.5243	117.0015
Temperature	C	30.58	34.08428
Pressure	BAR	2.58	2.58
Vapor Fraction		0	0
Liquid Fraction		1	1
Solid Fraction		0	0
Molar Enthalpy	CAL/MOL	11890.16	12007.46
Mass Enthalpy	CAL/GM	152.2162	153.7178
Enthalpy Flow	CAL/SEC	256146	258673
Molar Entropy	CAL/MOL-K	-59.81868	-59.43789
Mass Entropy	CAL/GM-K	-0.7657905	-0.7609156
Molar Density	MOL/CC	0.0110926	0.0110473
Mass Density	GM/CC	0.8664861	0.8629517
Average Molecular Weight	78.11364	78.11364	
Units	WATER	WO	

Stream Results H2

From			H2
To Substream: MIXED		H2	
Phase: Component Mole Flow		Vapor	Vapor
WATER	KMOL/HR	36.52455	36.52455
BENZENE	KMOL/HR	0	0
Mole Flow	KMOL/HR	36.52455	36.52455
Mass Flow	KG/HR	658	658
Volume Flow	L/MIN	2744.623	2605.568
Temperature	C	300.58	271.5121
Pressure	BAR	10.58	10.58
Vapor Fraction		1	1
Liquid Fraction		0	0
Solid Fraction		0	0
Molar Enthalpy	CAL/MOL	-55476.47	-55725.54
Mass Enthalpy	CAL/GM	-3079.412	-3093.238
Enthalpy Flow	CAL/SEC	-562850	-565380
Molar Entropy	CAL/MOL-K	-9.873431	-10.31892
Mass Entropy	CAL/GM-K	-0.5480587	-0.5727871
Molar Density	MOL/CC	0.000221795	0.000233631
Mass Density	GM/CC	0.00399569	0.00420894
Average Molecular Weight		18.01528	18.01528

HEATX (SHORTCUT METHOD) -Feed input same as heater, HEATX duty=10.58 KW



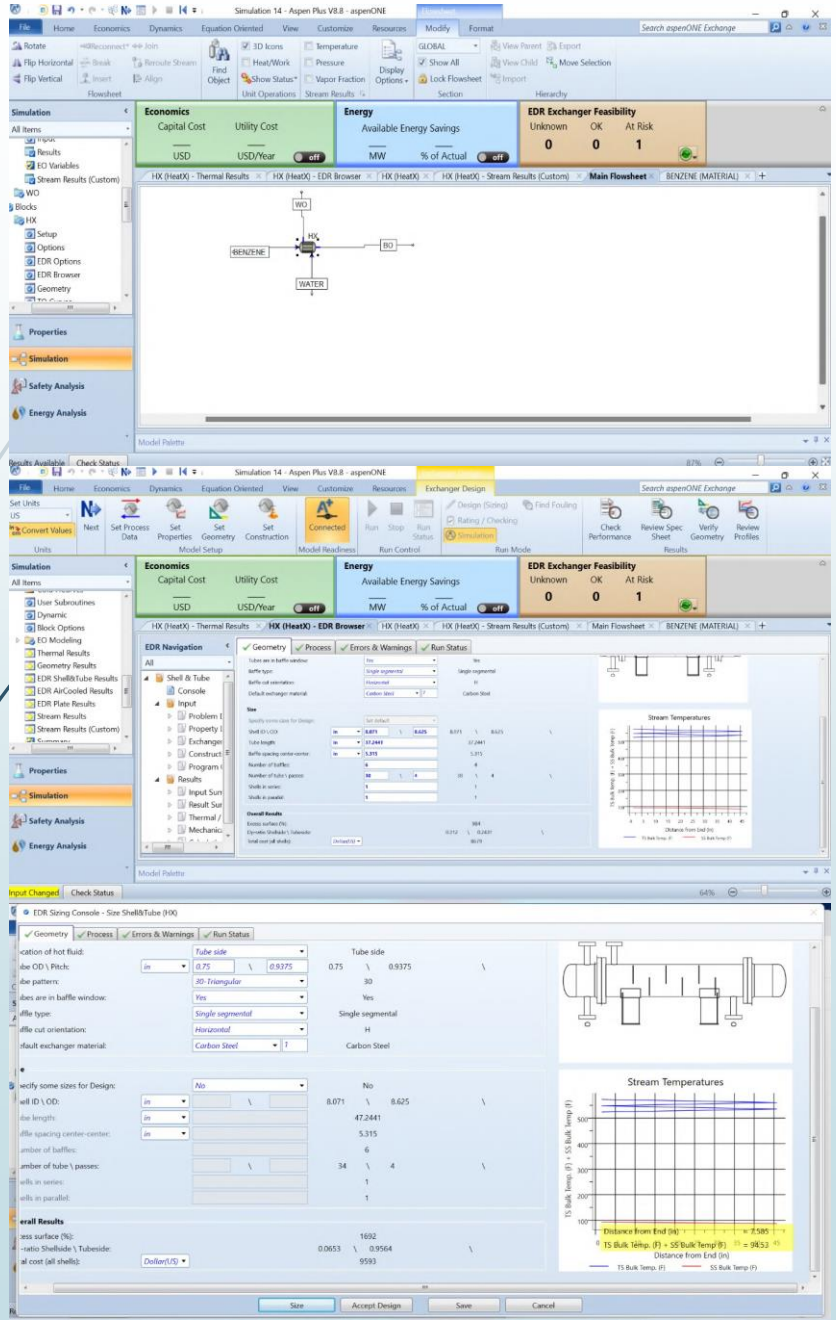


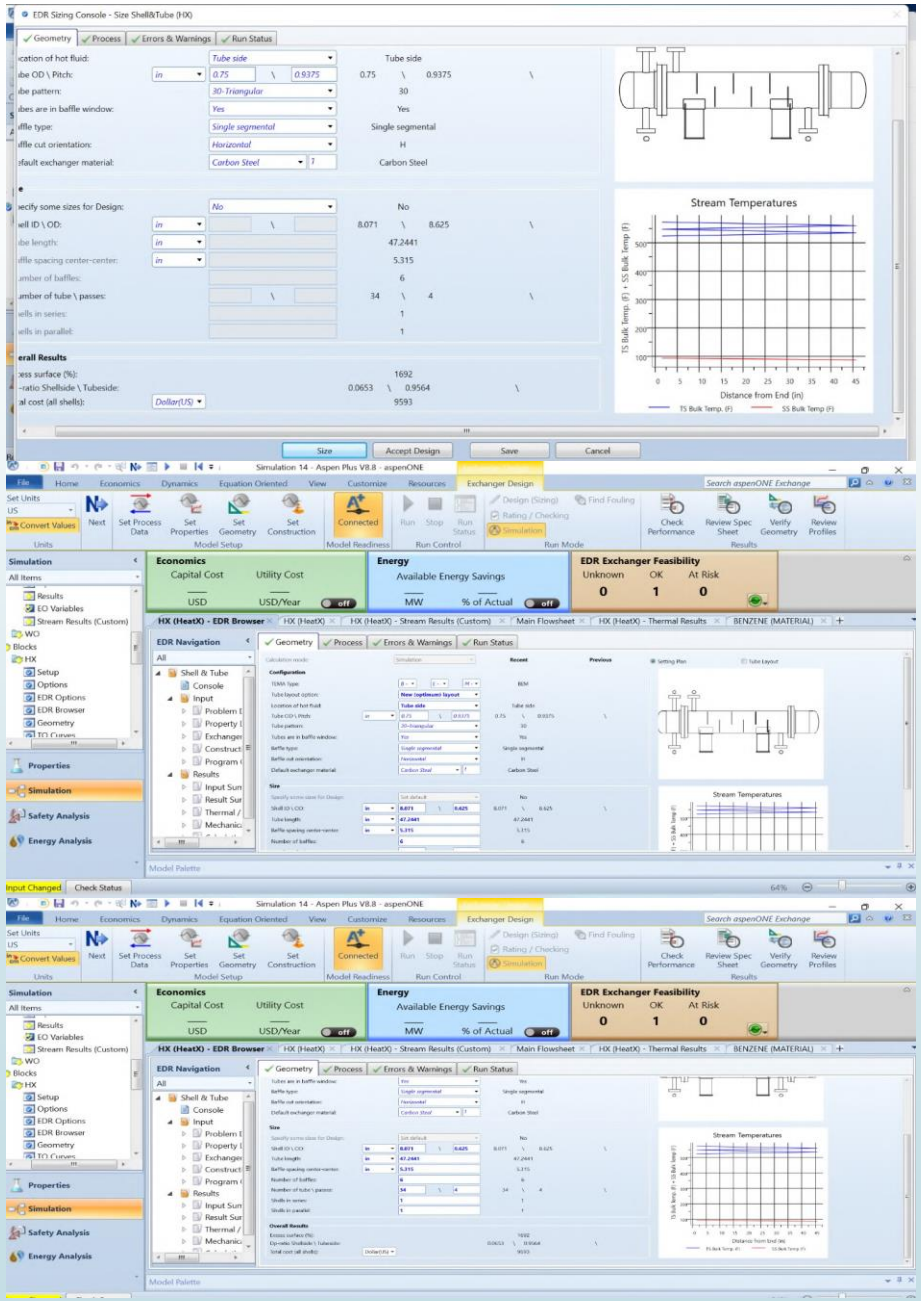
Stream Results

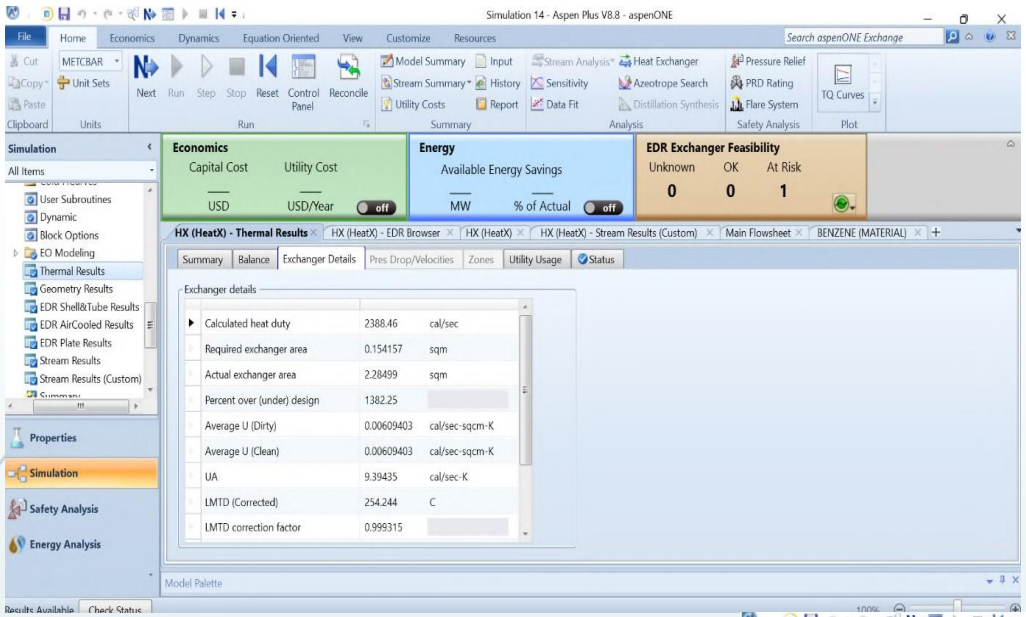
From		BENZENE	BO	WATER
To		HX	HX	HX
Substream: MIXED				
Phase:		Liquid	Liquid	Vapor
Component Mole Flow				
BENZENE	KMOL/HR	77.55368	77.55368	0
WATER	KMOL/HR	0	0	36.52455
Mole Flow	KMOL/HR	77.55368	77.55368	36.52455
Mass Flow	KG/HR	6058	6058	658
Volume Flow	L/MIN	116.5243	117.0015	2744.623
Temperature	C	30.58	34.08428	300.58
Pressure	BAR	2.58	2.58	10.58
Vapor Fraction		0	0	1
Liquid Fraction		1	1	0
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	11890.16	12007.46	-55476.47
Mass Enthalpy	CAL/GM	152.2162	153.7178	-3079.412
Enthalpy Flow	CAL/SEC	256146	258673	-562850
Molar Entropy	CAL/MOL-K	-59.81868	-59.43789	-9.873431
Mass Entropy	CAL/GM-K	-0.7657905	-0.7609156	-0.5480587
Molar Density	MOL/CC	0.0110926	0.0110473	0.000221795
Mass Density	GM/CC	0.8664861	0.8629517	0.00399569
Average Molecular Weight		78.11364	78.11364	18.01528

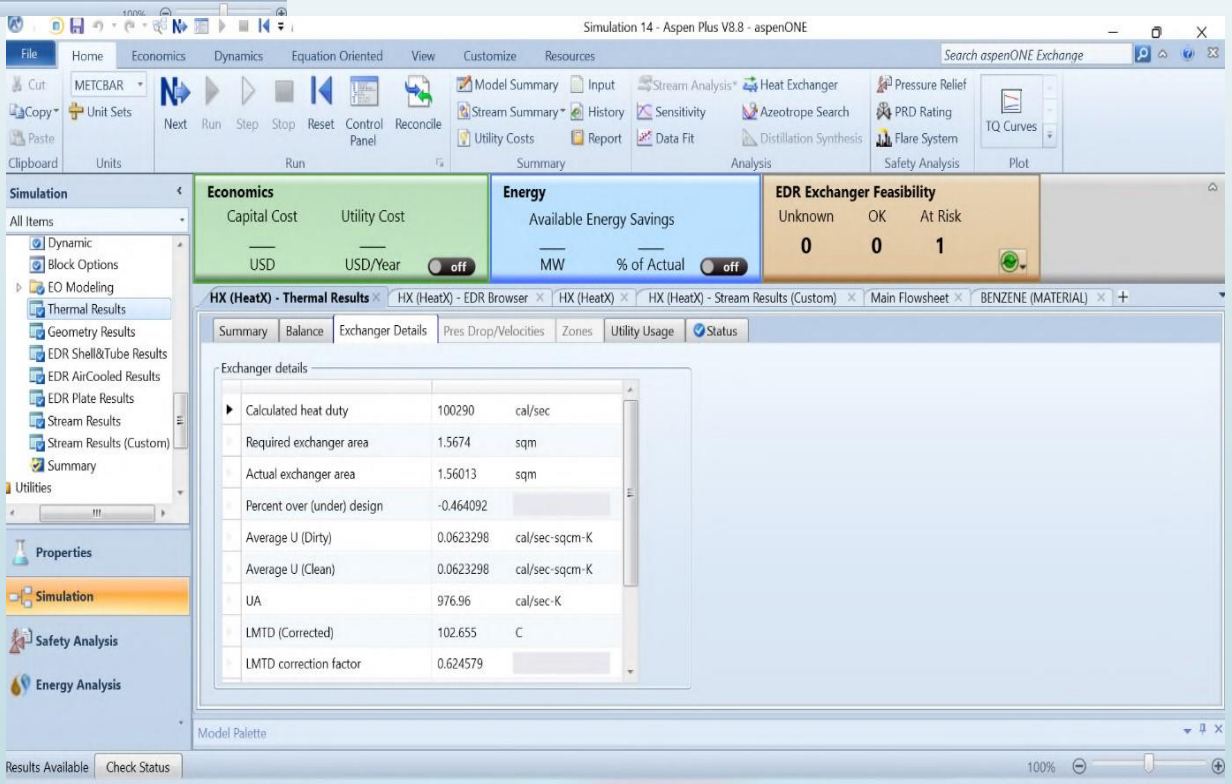
	Units	WO	
From		HX	
To			
Substream: MIXED			
Phase:		Vapor	
Component Mole Flow			
BENZENE	KMOL/HR	0	
WATER	KMOL/HR	36.52455	
Mole Flow	KMOL/HR	36.52455	
Mass Flow	KG/HR	658	
Volume Flow	L/MIN	2605.568	
Temperature	C	271.5121	
Pressure	BAR	10.58	
Vapor Fraction		1	
Liquid Fraction		0	
Solid Fraction		0	
Molar Enthalpy	CAL/MOL	-55725.54	
Mass Enthalpy	CAL/GM	-3093.238	
Enthalpy Flow	CAL/SEC	-565380	
Molar Entropy	CAL/MOL-K	-10.31892	
Mass Entropy	CAL/GM-K	-0.5727871	
Molar Density	MOL/CC	0.000233631	
Mass Density	GM/CC	0.00420894	
Average Molecular Weight		18.01528	

HEATX -SHELL AND TUBE METHOD






Simulation 14 - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
USD
USD/Year
Energy
Available Energy Savings
MW
% of Actual
EDR Exchanger Feasibility
Unknown
OK
At Risk
0
0
1
HX (HeatX) - Thermal Results
Exchanger details
Calculated heat duty 2388.46 cal/sec
Required exchanger area 0.154157 sqm
Actual exchanger area 2.28499 sqm
Percent over (under) design 1382.25
Average U (Dirty) 0.00609403 cal/sec-sqcm-K
Average U (Clean) 0.00609403 cal/sec-sqcm-K
UA 9.39435 cal/sec-K
LMTD (Corrected) 254.244 C
LMTD correction factor 0.999315


Simulation 14 - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
USD
USD/Year
Energy
Available Energy Savings
MW
% of Actual
EDR Exchanger Feasibility
Unknown
OK
At Risk
0
0
1
HX (HeatX) - Thermal Results
Exchanger details
Calculated heat duty 100290 cal/sec
Required exchanger area 1.5674 sqm
Actual exchanger area 1.56013 sqm
Percent over (under) design -0.464092
Average U (Dirty) 0.0623298 cal/sec-sqcm-K
Average U (Clean) 0.0623298 cal/sec-sqcm-K
UA 976.96 cal/sec-K
LMTD (Corrected) 102.655 C
LMTD correction factor 0.624579

Stream Results

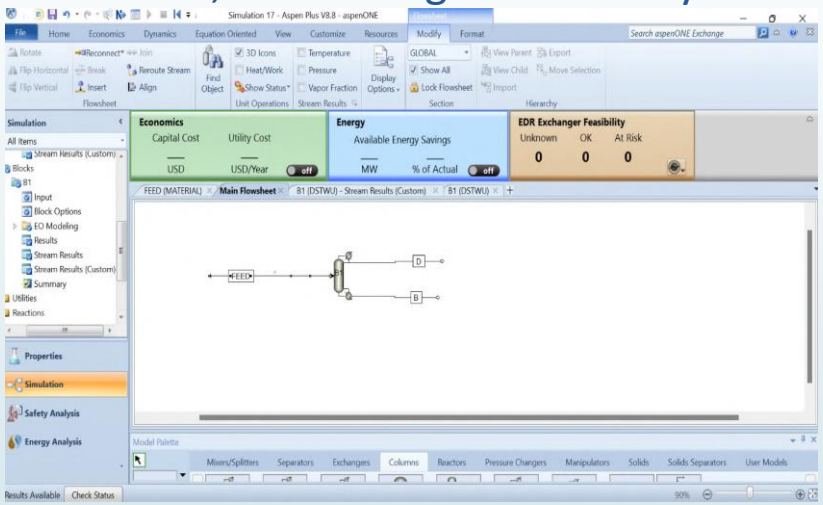
	Units	BENZENE	BO	WATER
From			HX	
To		HX		HX
Substream: MIXED Phase:		Liquid	Mixed	Vapor
Component Mole Flow				
BENZENE	KMOL/HR	77.55368	77.55368	0
WATER	KMOL/HR	0	0	36.52455
Mole Flow	KMOL/HR	77.55368	77.55368	36.52455
Mass Flow	KG/HR	6058	6058	658
Volume Flow	L/MIN	116.5243	11597.21	2744.623
Temperature	C	30.58	86.47616	300.58
Pressure	BAR	2.58	1.2271	10.58
Vapor Fraction		0	0.3656986	1
Liquid Fraction		1	0.6343014	0
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	11890.16	16545.57	-55476.47
Mass Enthalpy	CAL/GM	152.2162	211.8141	-3079.412
Enthalpy Flow	CAL/SEC	256146	356436	-562850
Molar Entropy	CAL/MOL-K	-59.81868	-46.49493	-9.873431
Mass Entropy	CAL/GM-K	-0.7657905	-0.5952217	-0.5480587
Molar Density	MOL/CC	0.0110926	0.000111455	0.000221795
Mass Density	GM/CC	0.8664861	0.00870612	0.00399569
Average Molecular Weight		78.11364	78.11364	

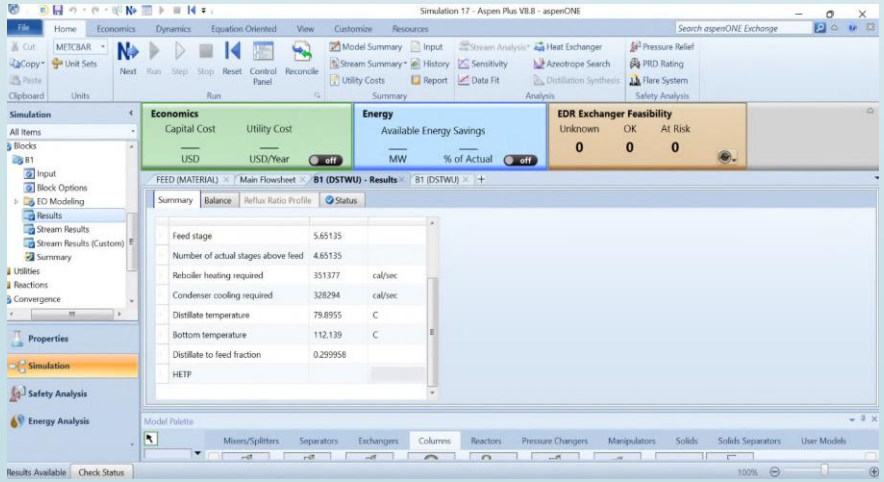
		WO
From		HX
To		
Substream: MIXED		
Phase:		Liquid
Component Mole Flow		
BENZENE	KMOL/HR	0
WATER	KMOL/HR	36.52455
Mole Flow	KMOL/HR	36.52455
Mass Flow	KG/HR	658
Volume Flow	L/MIN	13.08347
Temperature	C	171.2756
Pressure	BAR	10.5438
Vapor Fraction		0
Liquid Fraction		1
Solid Fraction		0
Molar Enthalpy	CAL/MOL	-65361.44
Mass Enthalpy	CAL/GM	-3628.111
Enthalpy Flow	CAL/SEC	-663140
Molar Entropy	CAL/MOL-K	-31.29548
Mass Entropy	CAL/GM-K	-1.737163
Molar Density	MOL/CC	0.0465276
Mass Density	GM/CC	0.8382079
Average Molecular Weight		18.01528

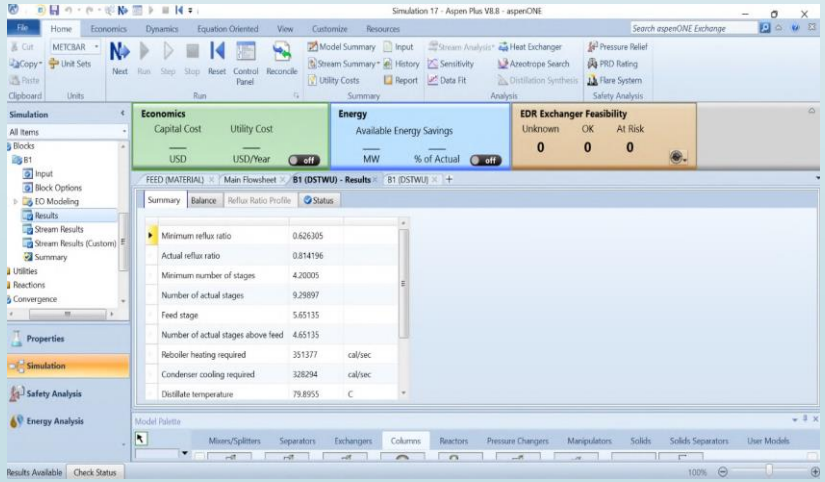
5). Columns (DSTWU, Distl, RadFrac) NRTL-RK Method

Feed – Methanol and Water(Pressure=18,98 psi, Saturated Liquid, Total flow rate=12058 lb/h with 0.368 and 0.632 mass fractions respectively

DSTWU – Pressure=1.58 atm(Both reboiler and condenser), Reflux Ratio=1.3 Rmin, Methanol recovery rate=0.981, 0.077 in light and heavy feed respectively



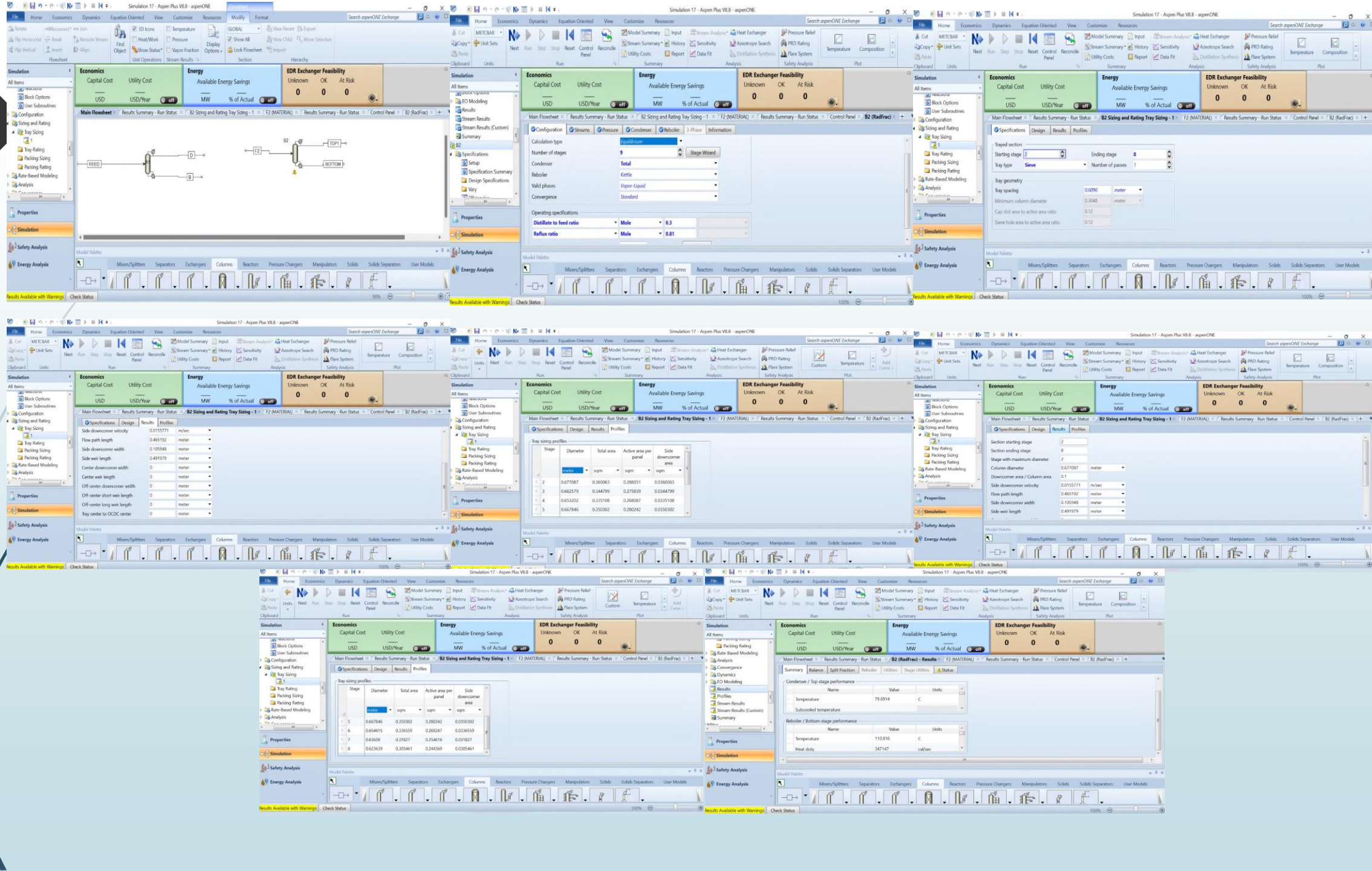




Stream Results				
	Units	B	D	FEED
From		B1	B1	
To				B1
Substream: MIXED Phase:				
Component Mole Flow				
METHANOL		Liquid	Liquid	Liquid
WATER				
Mole Flow	KMOL/HR	1.193495	61.62204	62.81553
Mass Flow	KMOL/HR	177.1001	14.77433	191.8744
Volume Flow	KMOL/HR	178.2936	76.39637	254.69
Temperature	KG/HR	3228.75	2240.667	5469.417
Pressure	L/MIN	59.67098	50.33995	109.1675
Vapor Fraction	C	112.1394	79.89553	87.46883
Liquid Fraction	BAR	1.600935	1.600935	1.308625
Solid Fraction		0	0	0
Molar Enthalpy		1	1	1
Mass Enthalpy		0	0	0
Enthalpy Flow	CAL/MOL	-66574.01	-57829.19	-64277.2
Molar Entropy	CAL/GM	-3676.258	-1971.708	-2993.145
Mass Entropy	CAL/SEC	-3297100	-1227200	-4547400
Molar Density	CAL/MOL-K	-34.31071	-49.15843	-39.06868 -1.81928 0.0388836
Mass Density	CAL/GM-K	-1.894659	-1.676075	0.8350192
Average Molecular Weight	MOL/CC	0.049799	0.0252934	21.4748
	GM/CC	0.9018203	0.7418452	
		18.10918	29.32949	

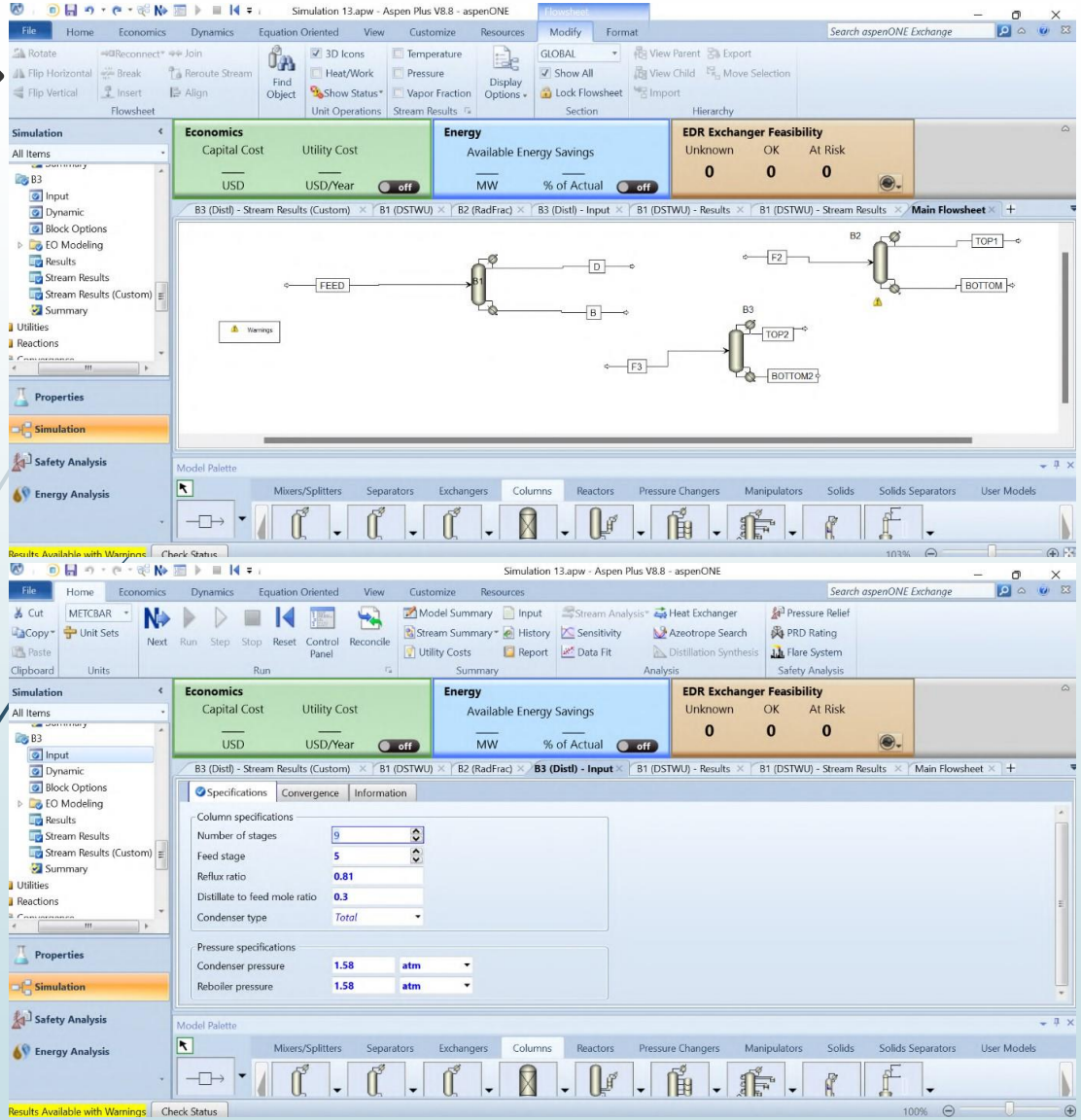
DSTWU Stream results

RADFRAC



		Stream results		
	Units	DBOTTOM	FEED2	
From		B12		BTOP1
To			B12	B12
Substream: MIXED Phase:		Liquid	Liquid	Liquid
Component Mole Flow				
METHANOL		2.5761.62204141	62.8155	62.150881.193495
WATER		14.7743374.6712	34 72302	177.10013.8 55
Mole Flow	KMOL/HR	177.2476.396373 32240.66729 1	191.874	178.293675.96143
Mass Flow	KMOL/HR	50.339959 84 53	488	23228.7540 249
Volume Flow	KMOL/HR	79.89553110.8161	4817	59.670 396098
Temperature	KG/HR	1.600935	254.693	79.69143112.1394
Pressure	L/MIN	0	2048	1.600935
Vapor Fraction	C	1	5469.41	0
Liquid Fraction	BAR	0	7	1
Solid Fraction		-665057829.1972	109.167	0
Molar Enthalpy		-36501971.7086 2	54 1	-5770066574.0117
Mass Enthalpy	CAL/MOL	-31227200746	87.4688	-1953676.258473
Enthalpy Flow	CAL/GM	-3449.158434 94 -1.676075891391	312739	-132971001 5
Molar Entropy	CAL/SEC	0.025293449358	1.30862	-4934.310714034
Mass Entropy	CAL/MOL-K	0.74184528992 6	5	-1.8946596751
Molar Density	CAL/GM-K	1829.3294921884	0	0.04979925121
Mass Density	MOL/CC		1	0.9018203740 687
Average Molecular Weight	GM/CC		0	2918.109184919
			- 64277.2 1 8 57	
			- 2993.1457 1 2	
			- 45474001 40	
			- 39.0686 822 22	
			- 1.81928 6057	

Distl – Input same as DSTWU



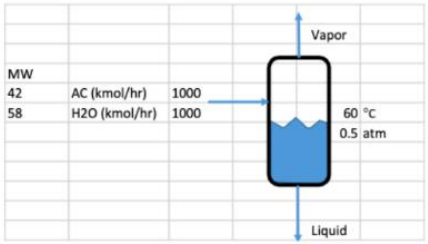
From To Substream: MIXED	Stream Results Units	BOTTOM2 B3	F3 B3	TOP2 B3
Phase: Component Mole Flow		Liquid	Liquid	Liquid
METHANOL	KMOL/HR	1.416167	62.81553	61.39937
WATER	KMOL/HR	176.867	191.8744	15.00739
Mole Flow	KMOL/HR	178.283	254.69	76.40699
Mass Flow	KG/HR	3231.682	5469.417	2237.737
Volume Flow	L/MIN	59.75223	109.1675	50.25661
Temperature	C	111.92	87.46883	79.94905
Pressure	BAR	1.600935	1.308625	1.600935
Vapor Fraction		0	0	0
Liquid Fraction		1	1	1
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	-66563.97	-64277.2	-57862.73
Mass Enthalpy	CAL/GM	-3672.151	-2993.145	-1975.709
Enthalpy Flow	CAL/SEC	-3296500	-4547400	-1228100
Molar Entropy	CAL/MOL-K	-34.33393	-39.06868	-49.09479
Mass Entropy	CAL/GM-K	-1.894108	-1.81928	-1.676329
Molar Density	MOL/CC	0.0497284	0.0388836	0.0253389
Mass Density	GM/CC	0.9014118	0.8350192	0.7421039
Average Molecular Weight		18.1267	21.4748	29.28708

ASSIGNMENT 2

Problem statement

(1) Design and sizing of a fresh drum (**Person 1**)

A stream with 1000kmol/hr of acetone (AC) and 1000kmol/hr of water (H2O) is fed into a flash drum. Vapor and liquid are separated at the drum.



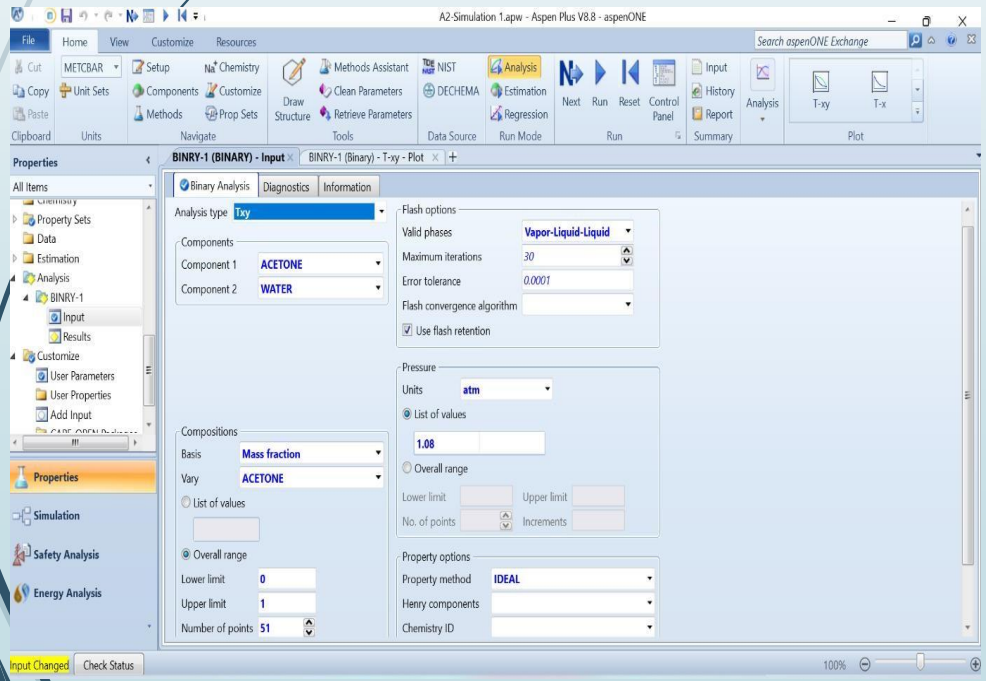
Assume ideal behaviour of the streams:

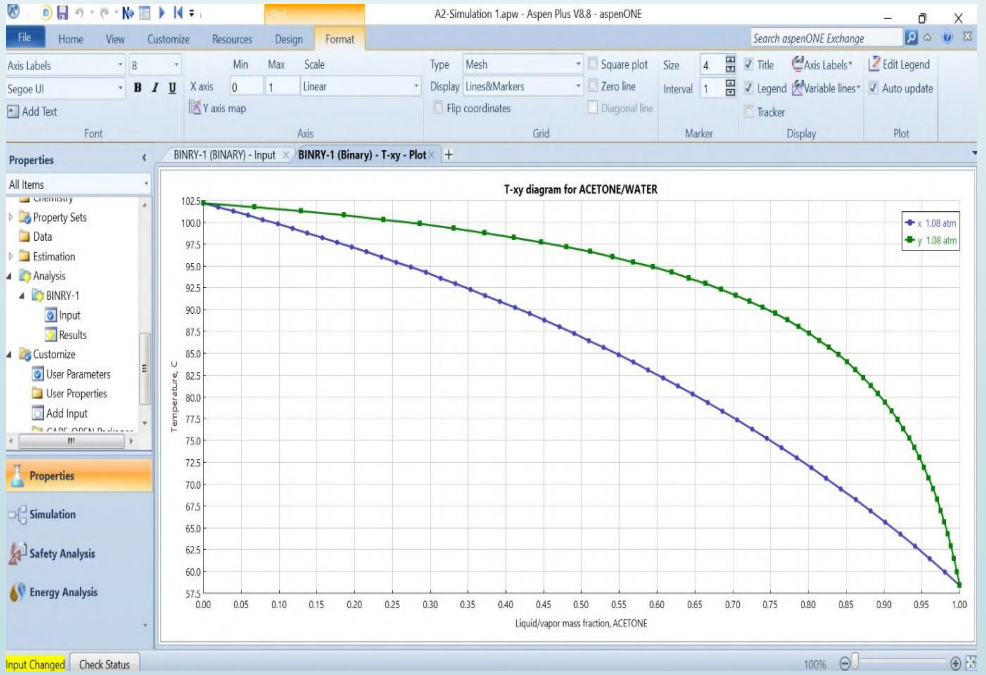
Q1: At 0.5 atm, to preform vapour-liquid separation, what are the maximum and minimum operating temperatures of the drum?

Q2: At 60°C and 0.5 atm,what are the vapour and liquid compositions and flow rates?

Hint Q1: Use Binary Analysis to find temperature range of 2 phase envelope

Solution- a) Maximum temperature=57.5 degree celcius, Minimum temperature=102.5 degree celcius

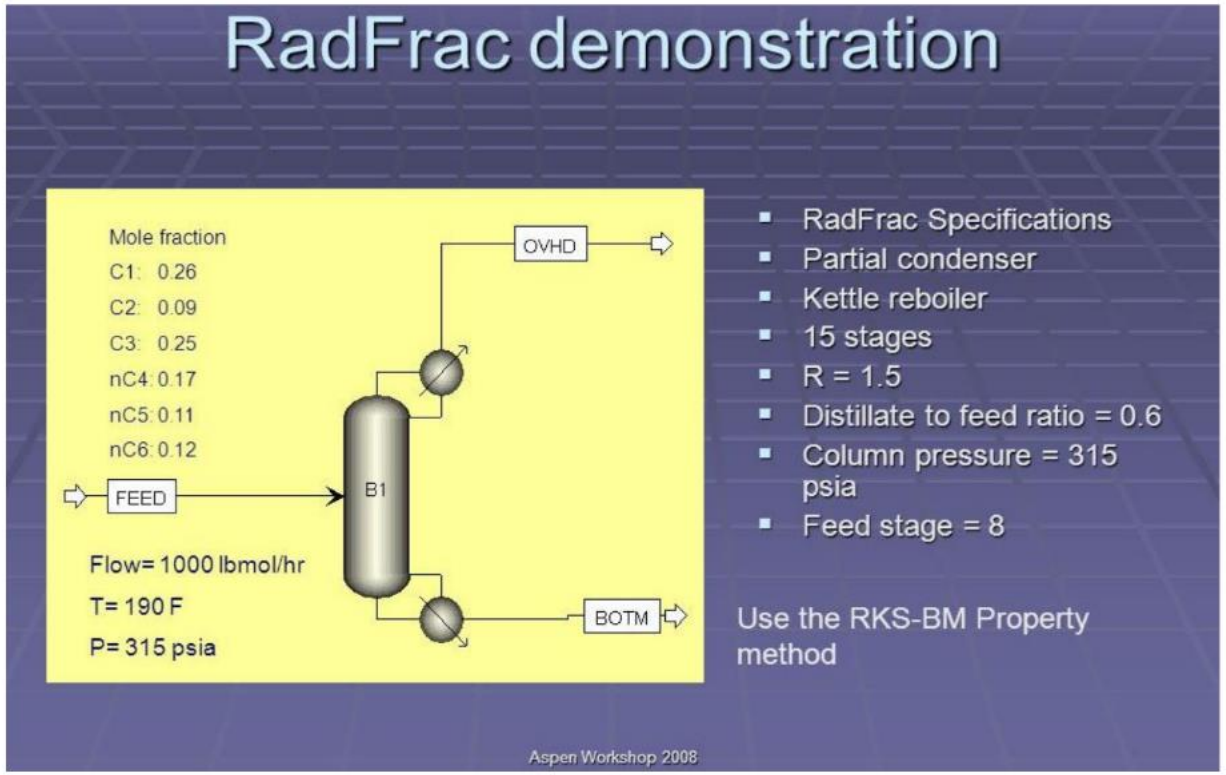




b)

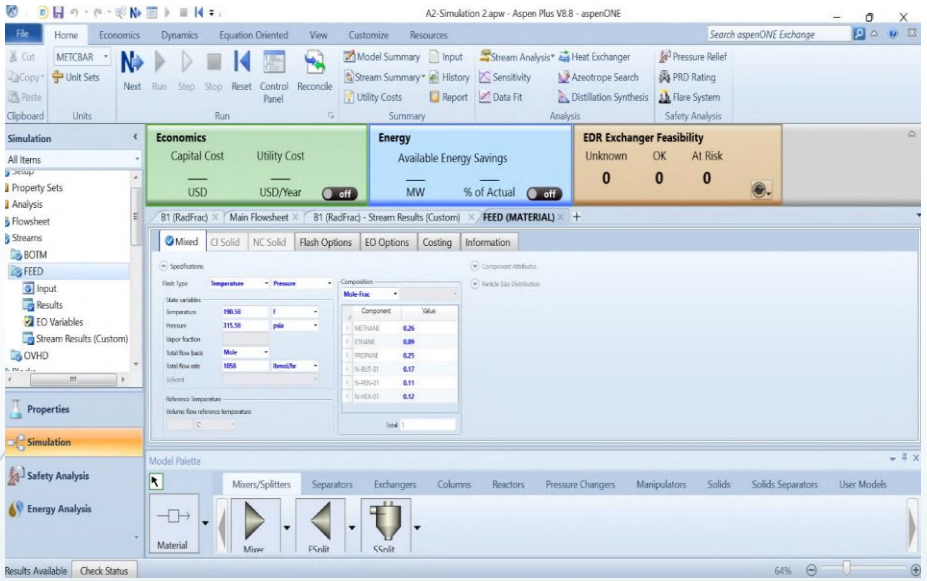
From To Substream: MIXED	Units	BOTM B1	FEED B1	OVHD B1
Phase: Component Mole Flow		Liquid	Mixed	Vapor
METHANE	KMOL/HR	7.67152E-05	124.7742	124.7741
ETHANE	KMOL/HR	0.0182493	43.19107	43.17282
PROPANE	KMOL/HR	4.65206	119.9752	115.3231
N-BUT-01	KMOL/HR	76.92444	81.58312	4.658679
N-PEN-01	KMOL/HR	52.77738	52.78908	0.0117031
N-HEX-01	KMOL/HR	57.58808	57.58809	4.25757E-06
Mole Flow	KMOL/HR	191.9603	479.9007	287.9404
Mass Flow	KG/HR	13447.48	22104.36	8656.884
Volume Flow	L/MIN	599.9331	6983.302	4507.856
Temperature	C	151.5982	88.1	23.35717
Pressure	BAR	21.75848	21.75848	21.75848
Vapor Fraction		0	0.7043279	1
Liquid Fraction		1	0.2956721	0
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	-34508.2	-26849.41	-21561.8
Mass Enthalpy	CAL/GM	-492.5982	-582.9188	-717.1767
Enthalpy Flow	CAL/SEC	-1840100	-3579200	-1724600
Molar Entropy	CAL/MOL-K	-108.916	-70.84468	-46.54626
Mass Entropy	CAL/GM-K	-1.554756	-1.538086	-1.548196
Molar Density	MOL/CC	0.00533283	0.00114535	0.00106459
Mass Density	GM/CC	0.3735827	0.0527552	0.0320066
Average Molecular Weight		70.05345	46.06028	30.06484

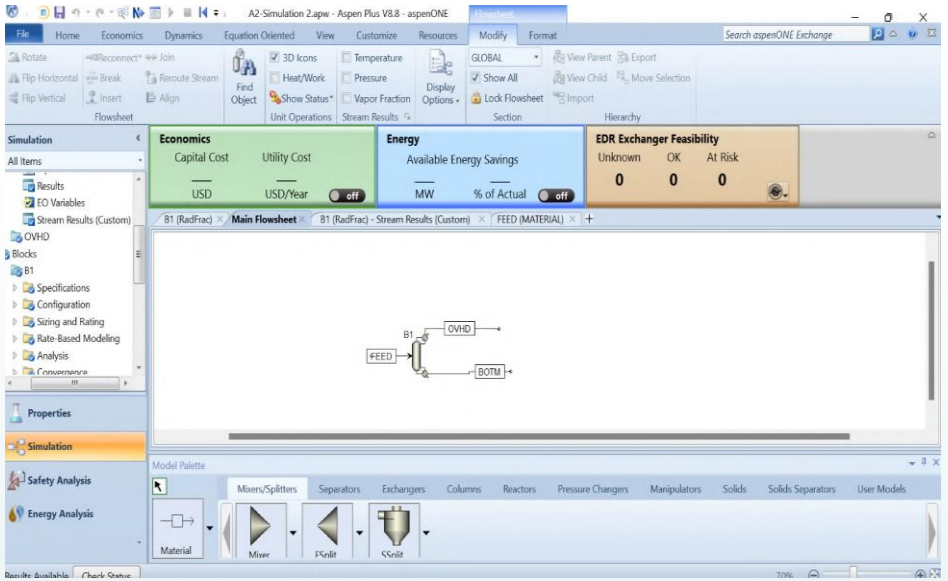
Q2).

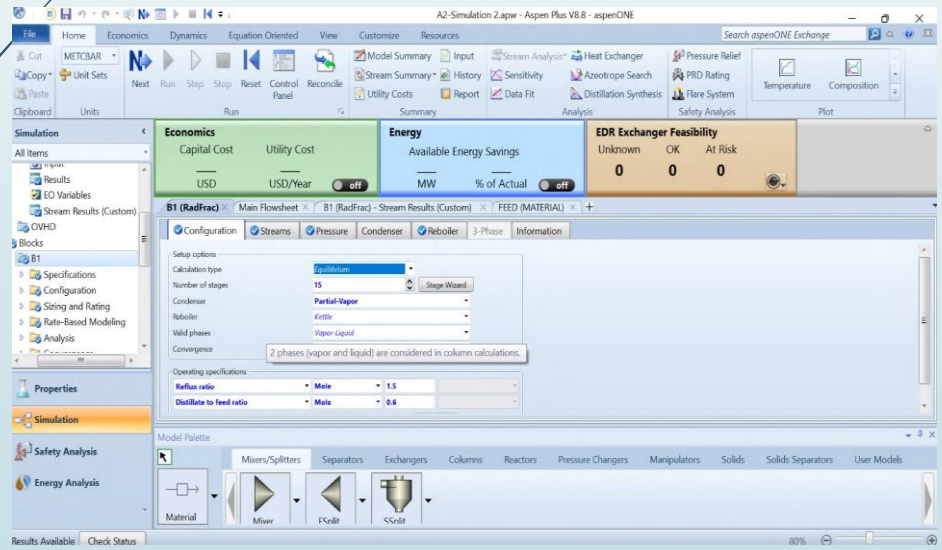


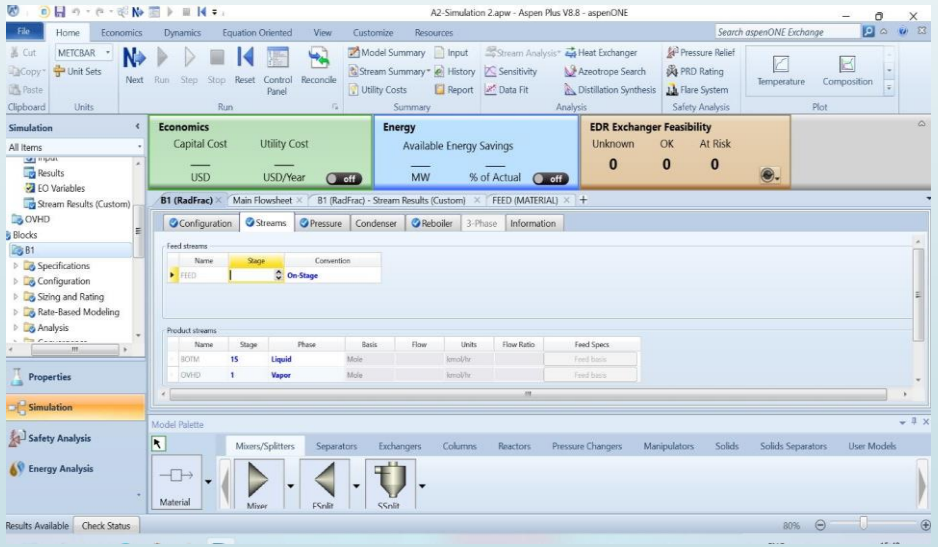
Here C1, C2……..nC6 represents hydrocarbons. Partial condenser means that distillate is coming out as vapor only.

Solution-


A2-Simulation 2.apw - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Unknown
OK
At Risk
B1 (RadFrac)
Main Flowsheet
B1 (RadFrac) - Stream Results (Custom)
FEED (MATERIAL)
Mixed
CI Solid
NC Solid
Flash Options
EO Options
Costing
Information
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
User Models
Material
Mixer
FSplit
SSplit
Properties
Simulation
Safety Analysis
Energy Analysis
Results Available
Check Status


A2-Simulation 2.apw - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Unknown
OK
At Risk
B1 (RadFrac)
Main Flowsheet
B1 (RadFrac) - Stream Results (Custom)
FEED (MATERIAL)
OVHD
FEED
BOTM
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
User Models
Material
Mixer
FSplit
SSplit
Properties
Simulation
Safety Analysis
Energy Analysis
Results Available
Check Status


A2-Simulation 2.apw - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Unknown
OK
At Risk
B1 (RadFrac)
Main Flowsheet
B1 (RadFrac) - Stream Results (Custom)
FEED (MATERIAL)
Configuration
Streams
Pressure
Condenser
Reboiler
3-Phase
Information
Setup options
Calculation type
Equilibrium
Number of stages
15
Stage Wizard
Condenser
Partial-Vapor
Reboiler
Kettle
Valid phases
Vapor-Liquid
Convergence
2 phases (vapor and liquid) are considered in column calculations.
Operating specifications
Reflux ratio
Mole
1.5
Distillate to feed ratio
Mole
0.6
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
User Models
Material
Mixer
FSplit
SSplit
Properties
Simulation
Safety Analysis
Energy Analysis
Results Available
Check Status


A2-Simulation 2.apw - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Unknown
OK
At Risk
B1 (RadFrac)
Main Flowsheet
B1 (RadFrac) - Stream Results (Custom)
FEED (MATERIAL)
Configuration
Streams
Pressure
Condenser
Reboiler
3-Phase
Information
Feed streams
Name
Stage
Convention
FEED
On-Stage
Product streams
Name
Stage
Phase
Basis
Flow
Units
Flow Ratio
Feed Specs
BOTM
15
Liquid
OVHD
1
Vapor
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
User Models
Material
Mixer
FSplit
SSplit
Properties
Simulation
Safety Analysis
Energy Analysis
Results Available
Check Status

Stream results

		Stream Results		
	Units	BOTM	FEED	OVHD
From		B1		B1
To			B1	
Substream: MIXED				
Phase:		Liquid	Mixed	Vapor
Component Mole Flow				
METHANE	KMOL/HR	7.67009E-05	124.7742	124.7741
ETHANE	KMOL/HR	0.0182474	43.19107	43.17282
PROPANE	KMOL/HR	4.651484	119.9752	115.3237
N-BUT-01	KMOL/HR	76.92502	81.58312	4.658109
N-PEN-01	KMOL/HR	52.77738	52.78908	0.0116956
N-HEX-01	KMOL/HR	57.58808	57.58809	4.25115E-06
Mole Flow	KMOL/HR	191.9603	479.9007	287.9404
Mass Flow	KG/HR	13447.49	22104.36	8656.875
Volume Flow	L/MIN	599.9341	6983.302	4507.852
Temperature	C	151.5985	88.1	23.35694
Pressure	BAR	21.75848	21.75848	21.75848
Vapor Fraction		0	0.7043279	1
Liquid Fraction		1	0.2956721	0
Solid Fraction		0	0	0
Molar Enthalpy	CAL/MOL	-34508.2	-26849.41	-21561.79
Mass Enthalpy	CAL/GM	-492.5979	-582.9188	-717.1771
Enthalpy Flow	CAL/SEC	-1840100	-3579200	-1724600
Molar Entropy	CAL/MOL-K	-108.9161	-70.84468	-46.54624
Mass Entropy	CAL/GM-K	-1.554756	-1.538086	-1.548196
Molar Density	MOL/CC	0.00533282	0.00114535	0.00106459
Mass Density	GM/CC	0.3735823	0.0527552	0.0320066
Average Molecular Weight		70.05349	46.06028	30.06481

Question 3

(25 pts) Aspen PLUS problem--REquil Reactor: Consider the reaction to produce two ethylbenzene molecules from one molecule each of diethylbenzene and benzene. The reaction equation is as follows:

$$C_{10}H_{14} + C_6H_6 \rightarrow 2\,C_8H_{10}$$

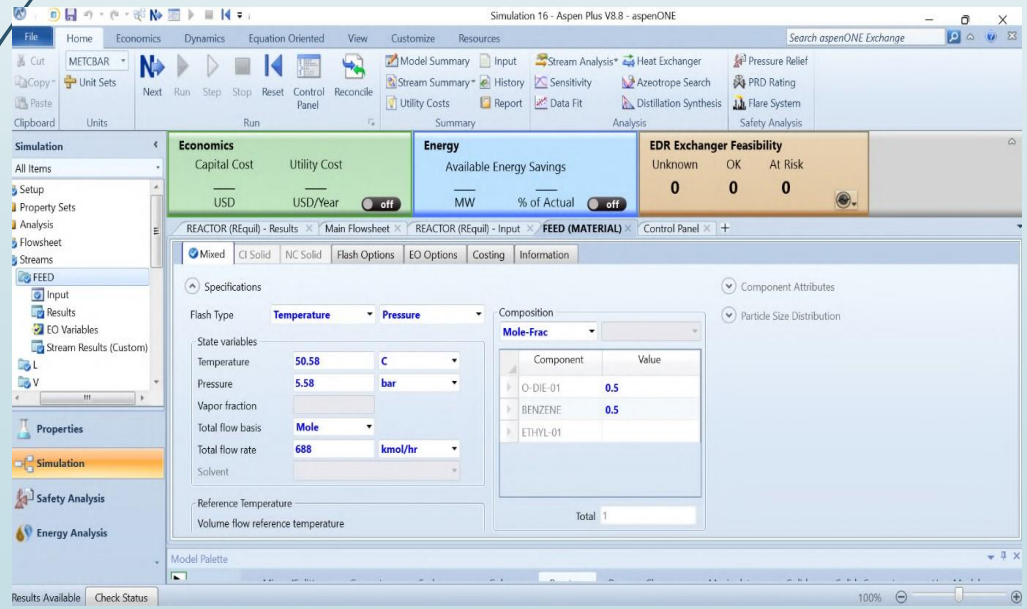
Diethylbenzene (DIEB) + Benzene → 2 Ethylbenzene

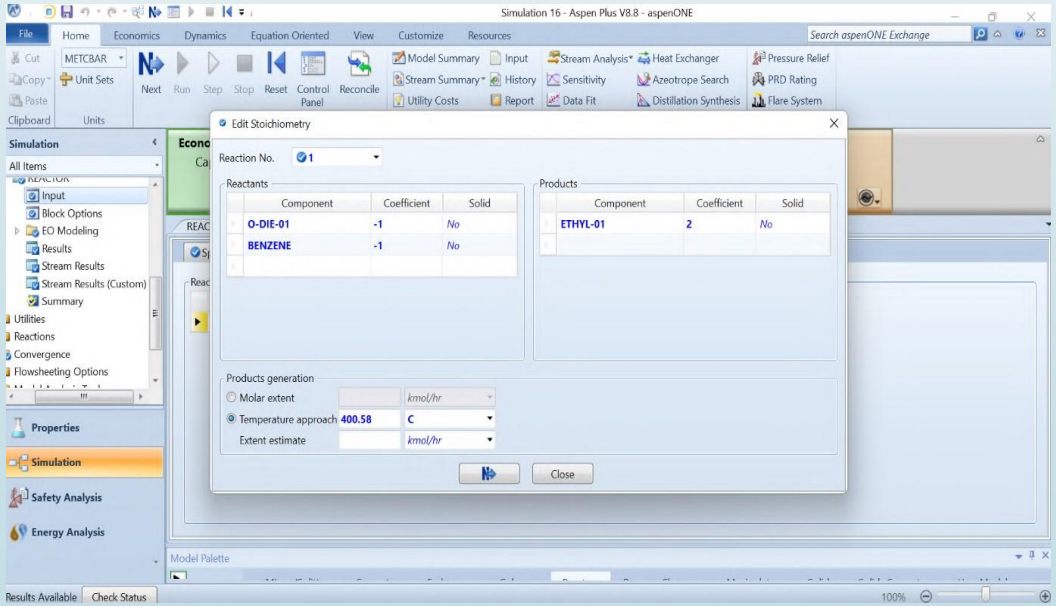
The objective for this problem is to simulate this reaction using an REquil reactor in Aspen PLUS. The feed to the system is at 50 °C and 5 bar, and consists of a total flow of 630 kg moles/hr of an equimolar mix of the two reactants.

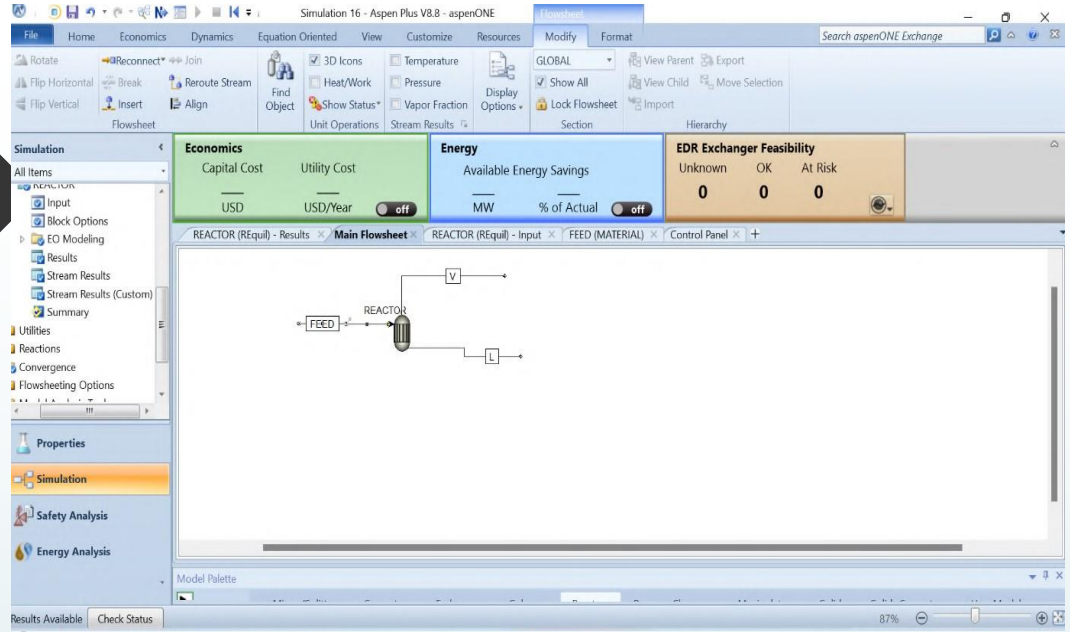
- Use method as Peng-Rob
- Operating temperature and pressure of reactor are 200 °C and 5 bar
- Take approach temperature as 400 °C

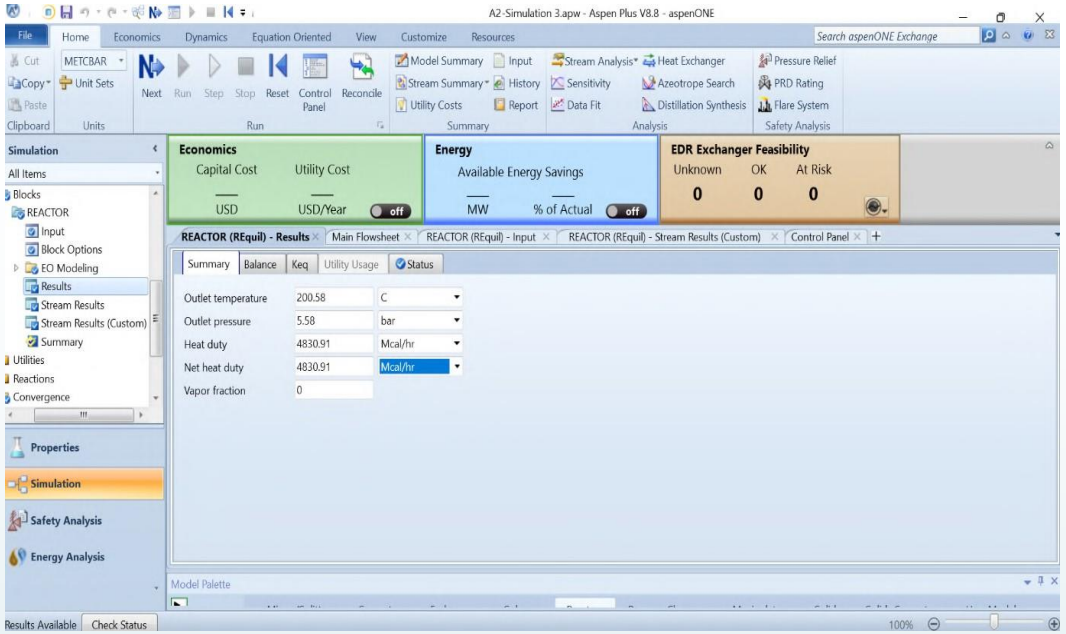
Also find conversion of benzene, vapor fraction and net heat duty in Mcal/hr.

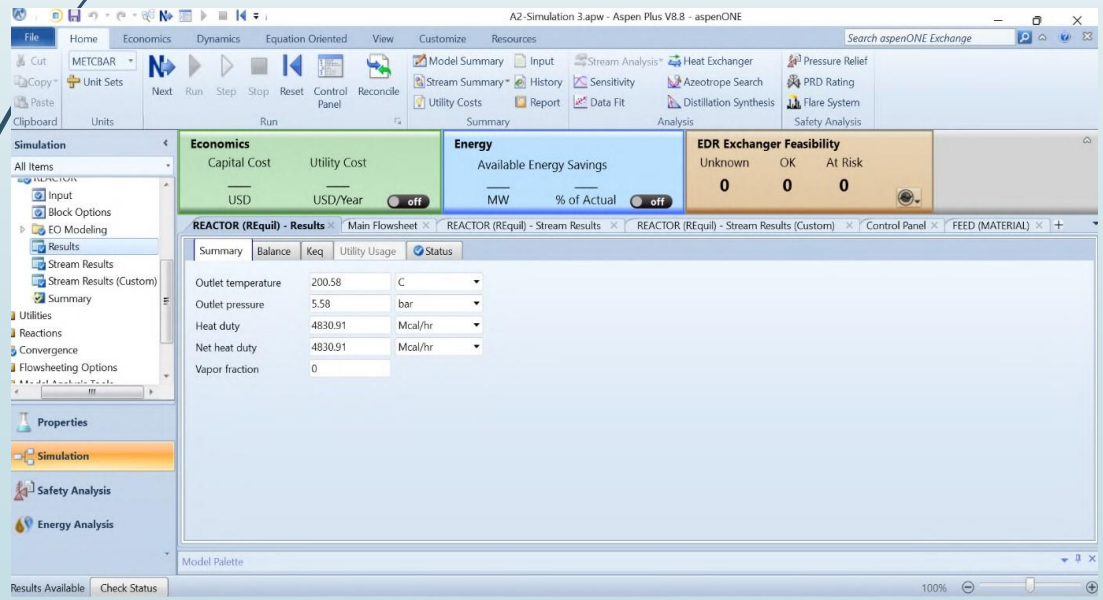
Solution






Simulation 16 - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Unknown
OK
At Risk
REACTOR
FEED
V
L


A2-Simulation 3.apw - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Outlet temperature 200.58 C
Outlet pressure 5.58 bar
Heat duty 4830.91 Mcal/hr
Net heat duty 4830.91 Mcal/hr
Vapor fraction 0


A2-Simulation 3.apw - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Outlet temperature 200.58 C
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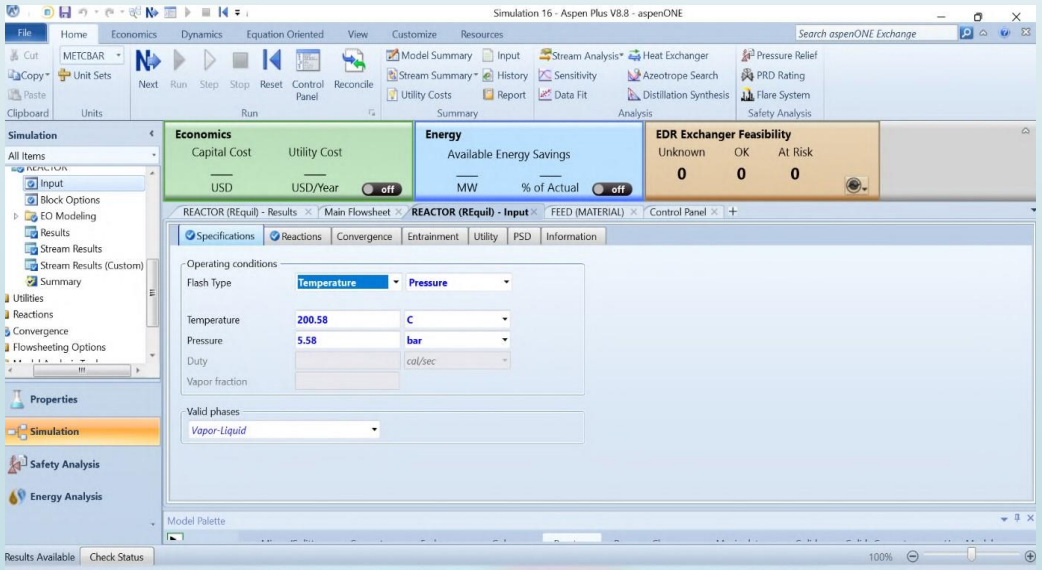
Heat duty 4830.91 Mcal/hr
Net heat duty 4830.91 Mcal/hr
Vapor fraction 0


Simulation 16 - Aspen Plus V8.8 - aspenONE
Economics
Capital Cost
Utility Cost
Energy
Available Energy Savings
EDR Exchanger Feasibility
Operating conditions
Flash Type Temperature Pressure
Temperature 200.58 C
Pressure 5.58 bar
Duty cal/sec
Vapor fraction
Valid phases
Vapor-Liquid

Net heat duty=4830.91 Mcal/hr

Vapour fraction=0

	Units	FEED	L	V
From			REACTOR	REACTOR
To Substream: MIXED		REACTOR		
Phase: Component Mole Flow		Liquid	Liquid	Missing
O-DIE-01	KMOL/HR	344	112.3756	0
BENZENE	KMOL/HR	344	112.3756	0
ETHYL-01	KMOL/HR	0	463.2489	0
Mole Flow	KMOL/HR	688	688	0
Mass Flow	KG/HR	73043.17	73043.17	0
Volume Flow	L/MIN	1454.104	1766.143	0
Temperature	C	50.58	200.58	
Pressure	BAR	5.58	5.58	5.58
Vapor Fraction		0	0	
Liquid Fraction		1	1	
Solid Fraction		0	0	
Molar Enthalpy	CAL/MOL	-372.096	6649.575	
Mass Enthalpy	CAL/GM	-3.504805	62.63293	
Enthalpy Flow	CAL/SEC	-71111.68	1270810	
Molar Entropy	CAL/MOL-K	-101.6332	-80.73425	
Mass Entropy	CAL/GM-K	-0.9572916	-0.760443	
Molar Density	MOL/CC	0.00788573	0.00649249	
Mass Density	GM/CC	0.8372073	0.6892907	
Average Molecular Weight		106.1674	106.1674	

Thank You