SimuTech Project

REPORT ON: PROCESS SIMULATION AND MODELLING IN ASPEN PLUS

REPORT BY SANDEEP PAL

PROJECT MENTOR :-
Nishesh Jyoti

Objective :-

- Aspen Plus is a process modeling tool used for process monitoring, optimization and conceptual design, especially by chemical process industries . Main objective of this project is learn simulate the basic flowsheet and process design in Aspen plus and to learn the important features of Aspen plus.

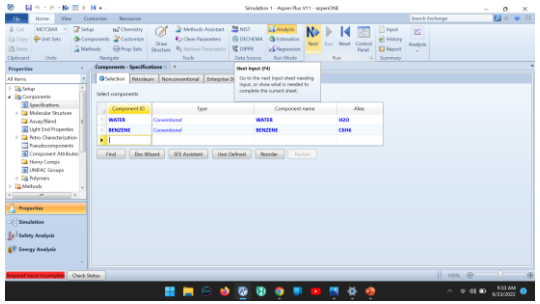
Acknowledgement

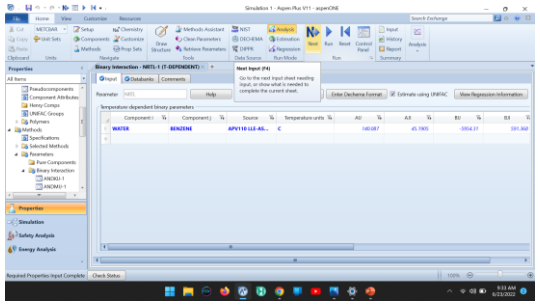
- I would like to express my special thanks of gratitude to my Mentor Nishesh Jyoti who gave me the golden opportunity to do this project on the topic process simulation and modelling in aspen plus. It helped me in doing a lot of Research and i came to know about a lot of things related to this topic.

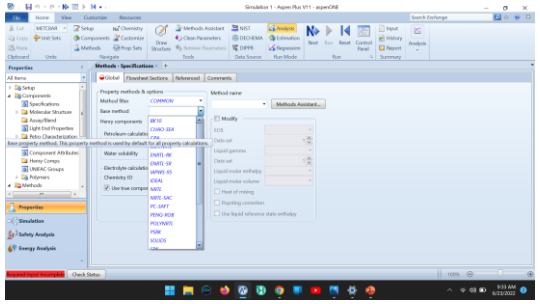
Introduction

ASPEN is a process simulation software package widely used in industry. Given a process design and an appropriate selection of thermodynamic models, ASPEN uses mathematical models to predict the performance of the process. This information can then be used in an iterative fashion to optimize the design.

ASPEN *does not* design the process. It takes a design that the user supplies and *simulates the performance* of the process specified in that design. Therefore, a solid understanding of the underlying chemical engineering principles is required to supply reasonable values of input parameters and to evaluate the suitability of the results obtained. For instance, a user should have some idea of the column behavior before attempting to use ASPEN. This information could come from an approximate method

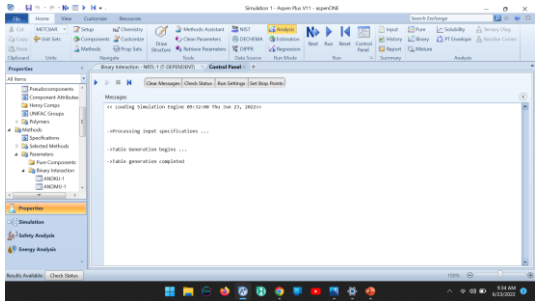


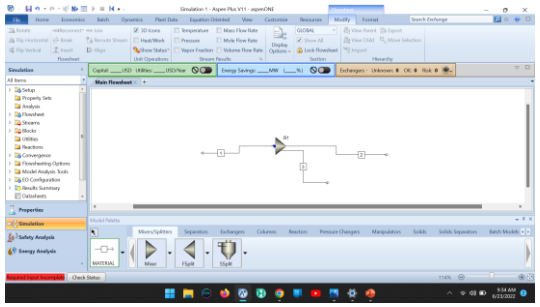


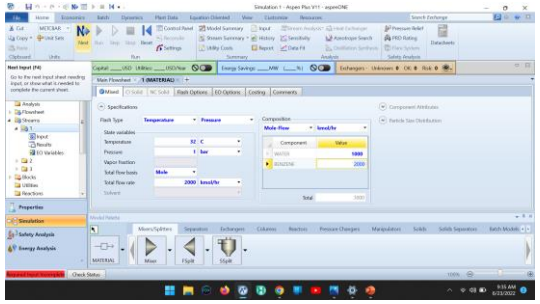


Steps to produce a simulation

- Select the simulation type a blank batch process.
- Specify the component by either entering the chemical formula for by name .
- If your formula is available in general the use find button to specify your compound.
- Next click on next button to proceed further.
- Select the base method for calculation of properties like NRTL , NRTL-RK , IDEAL etc.
- Wait for aspen to calculate the data.

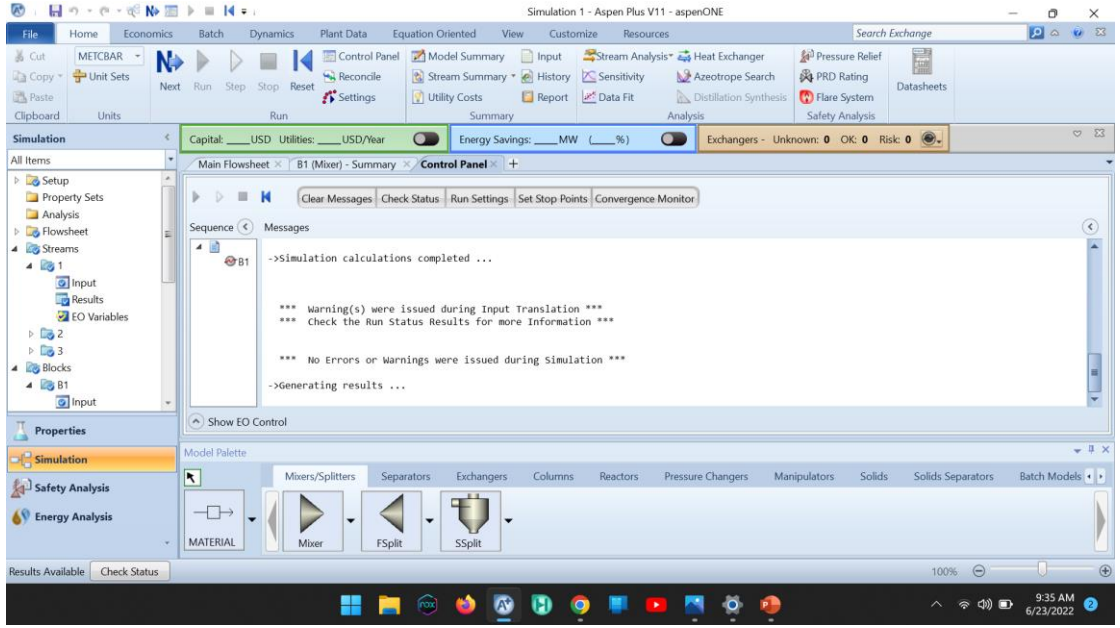


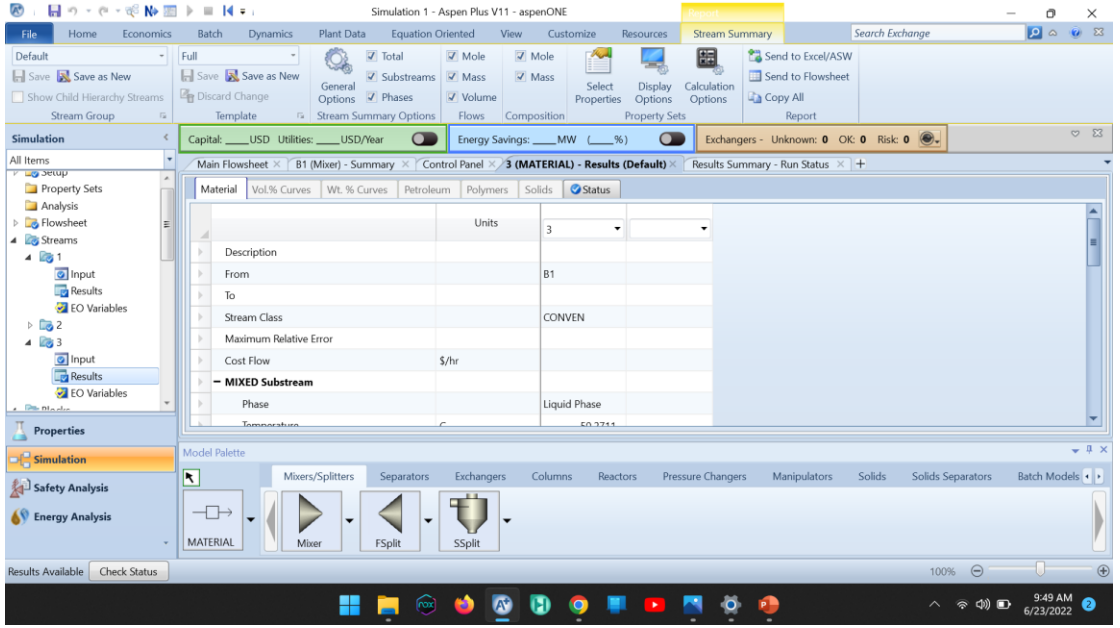




Simulation

- after estimating the properties go to simulation section and ad the device and component required for the process.
- Add the input and output stream of the device used.
- Devices are operated at certain properties specify the properties like temperature , pressure etc and also specify the input stream operating properties.
- Click on next and generate the results as shown.
- Results of the output stream can be seen at the right side of the screen.


Simulation 1 - Aspen Plus V11 - aspenONE
File
Home
Economics
Batch
Dynamics
Plant Data
Equation Oriented
View
Customize
Resources
Search Exchange
Next
Run
Step
Stop
Reset
Control Panel
Reconcile
Settings
Model Summary
Stream Summary
Utility Costs
Input
History
Report
Stream Analysis
Sensitivity
Data Fit
Heat Exchanger
Azeotrope Search
Distillation Synthesis
Pressure Relief
PRD Rating
Flare System
Datasheets
Simulation
All Items
Setup
Property Sets
Analysis
Flowsheet
Streams
1
Input
Results
EO Variables
2
3
Blocks
B1
Input
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Exchangers - Unknown: 0 OK: 0 Risk: 0
Main Flowsheet
B1 (Mixer) - Summary
Control Panel
Clear Messages
Check Status
Run Settings
Set Stop Points
Convergence Monitor
Sequence
Messages
->Simulation calculations completed ...
*** Warning(s) were issued during Input Translation ***
*** Check the Run Status Results for more Information ***
*** No Errors or Warnings were issued during Simulation ***
->Generating results ...
Show EO Control
Properties
Simulation
Safety Analysis
Energy Analysis
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
Batch Models
MATERIAL
Mixer
FSplit
SSplit
Results Available
Check Status
100%
9:35 AM
6/23/2022

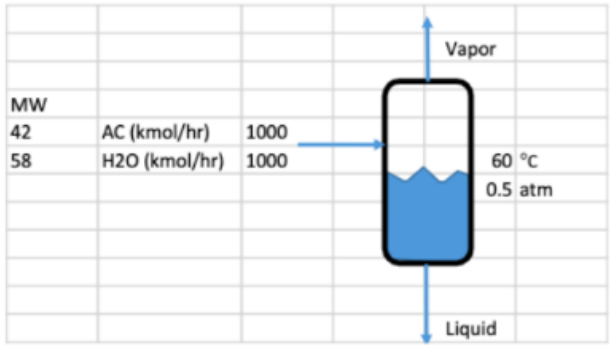

Simulation 1 - Aspen Plus V11 - aspenONE
File
Home
Economics
Batch
Dynamics
Plant Data
Equation Oriented
View
Customize
Resources
Stream Summary
Search Exchange
Default
Full
Save
Save as New
Discard Change
Show Child Hierarchy Streams
Stream Group
Template
General Options
Total
Substreams
Phases
Stream Summary Options
Mole
Mass
Volume
Flows
Composition
Select Properties
Display Options
Calculation Options
Property Sets
Send to Excel/ASW
Send to Flowsheet
Copy All
Report
Simulation
All Items
Property Sets
Analysis
Flowsheet
Streams
1
Input
Results
EO Variables
2
3
Input
Results
EO Variables
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Exchangers - Unknown: 0 OK: 0 Risk: 0
Main Flowsheet
B1 (Mixer) - Summary
Control Panel
3 (MATERIAL) - Results (Default)
Results Summary - Run Status
Material
Vol.% Curves
Wt. % Curves
Petroleum
Polymers
Solids
Status
Units
3
Description
From
B1
To
Stream Class
CONVEN
Maximum Relative Error
Cost Flow
$/hr
MIXED Substream
Phase
Liquid Phase
Properties
Simulation
Safety Analysis
Energy Analysis
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
Batch Models
MATERIAL
Mixer
FSplit
SSplit
Results Available
Check Status
100%
9:49 AM
6/23/2022

Assignment

- Problem 1 :-

(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 dru
Vapor and liquid are separated at the drum.



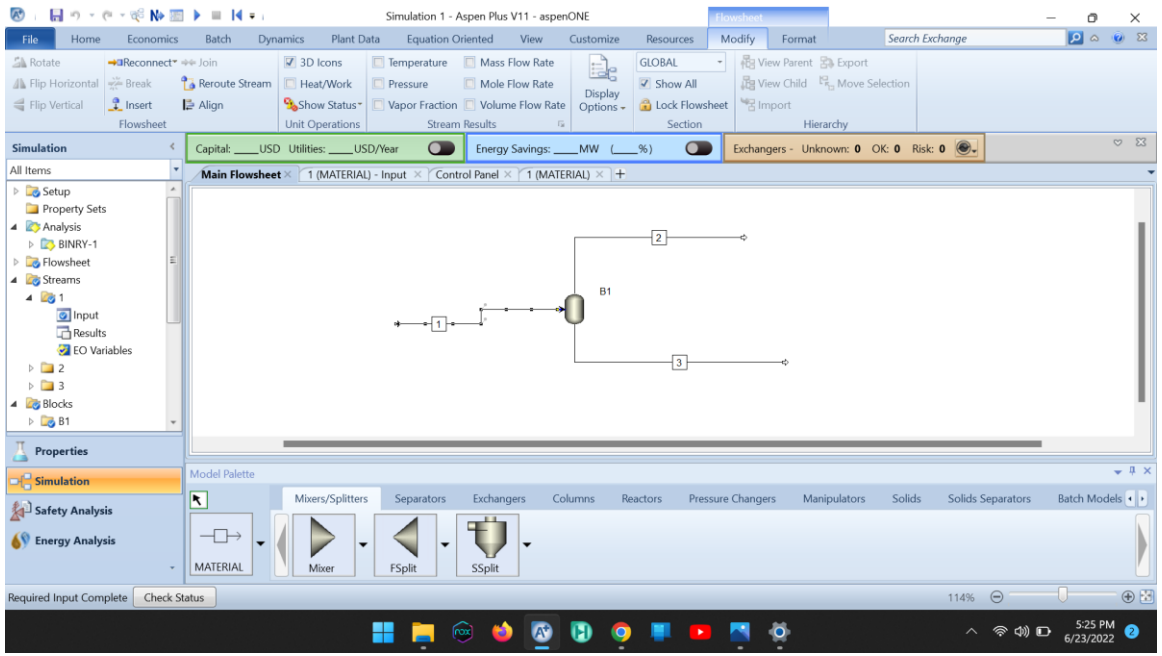
Assume ideal behaviour of the streams:

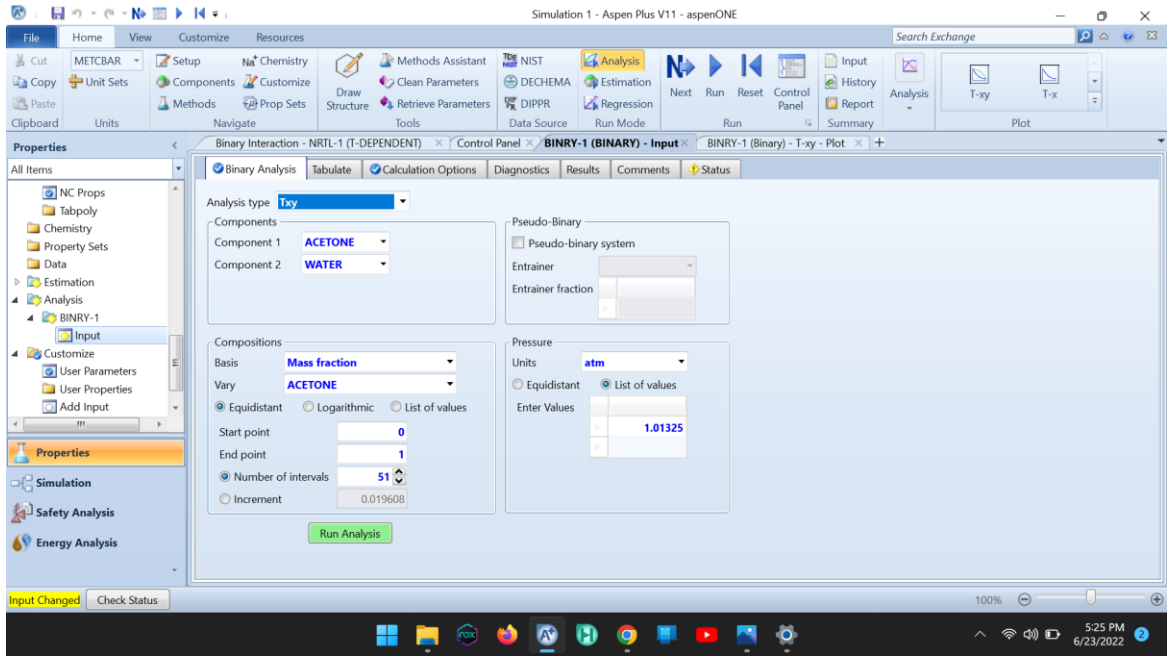
Q1: At 0.5 atm, to preform vapour-liquid separation, what are the maximum and minimum operating temperatures of the drum?

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

Solution

- 1)


Simulation 1 - Aspen Plus V11 - aspenONE
Main Flowsheet
1 (MATERIAL) - Input
Control Panel
1 (MATERIAL)
B1
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
Batch Models
MATERIAL
Mixer
FSplit
SSplit
Required Input Complete
Check Status
5:25 PM
6/23/2022

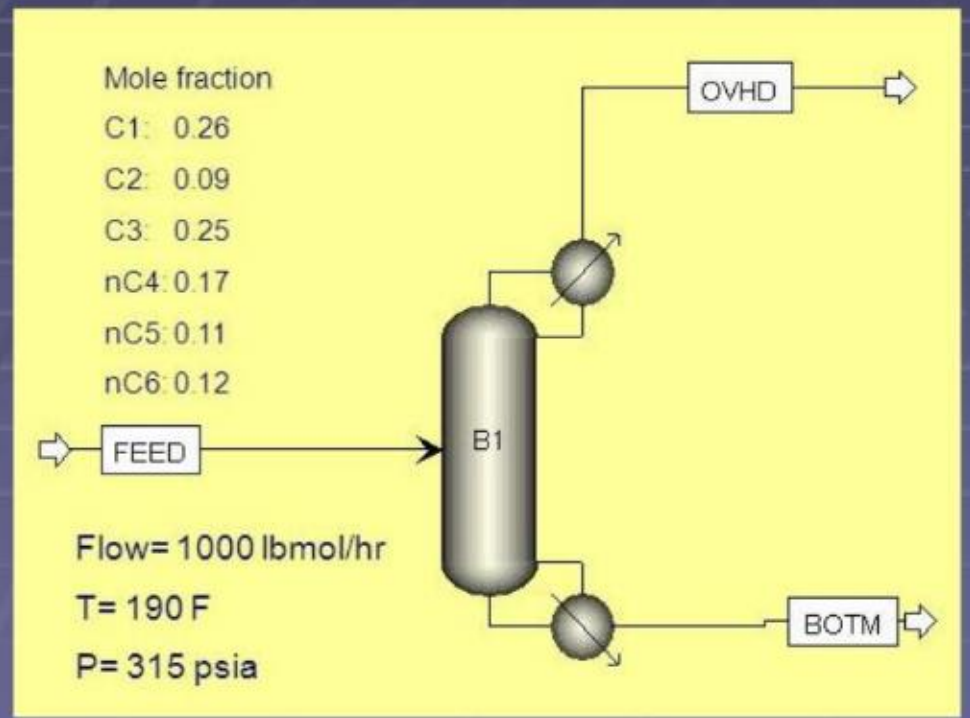

Simulation 1 - Aspen Plus V11 - aspenONE
Binary Interaction - NRTL-1 (T-DEPENDENT)
Control Panel
BINRY-1 (BINARY) - Input
BINRY-1 (Binary) - T-xy - Plot
Binary Analysis
Tabulate
Calculation Options
Diagnostics
Results
Comments
Status
Analysis type
Txy
Components
Component 1
ACETONE
Component 2
WATER
Pseudo-Binary
Pseudo-binary system
Entrainer
Entrainer fraction
Compositions
Basis
Mass fraction
Vary
ACETONE
Equidistant
Logarithmic
List of values
Start point
0
End point
1
Number of intervals
51
Increment
0.019608
Pressure
Units
atm
Equidistant
List of values
Enter Values
1.01325
Run Analysis
Input Changed
Check Status
5:25 PM
6/23/2022

Minimum operating tem. = 56.5 degree Celsius

Maximum operating tem.= 100.1 degree Celsius

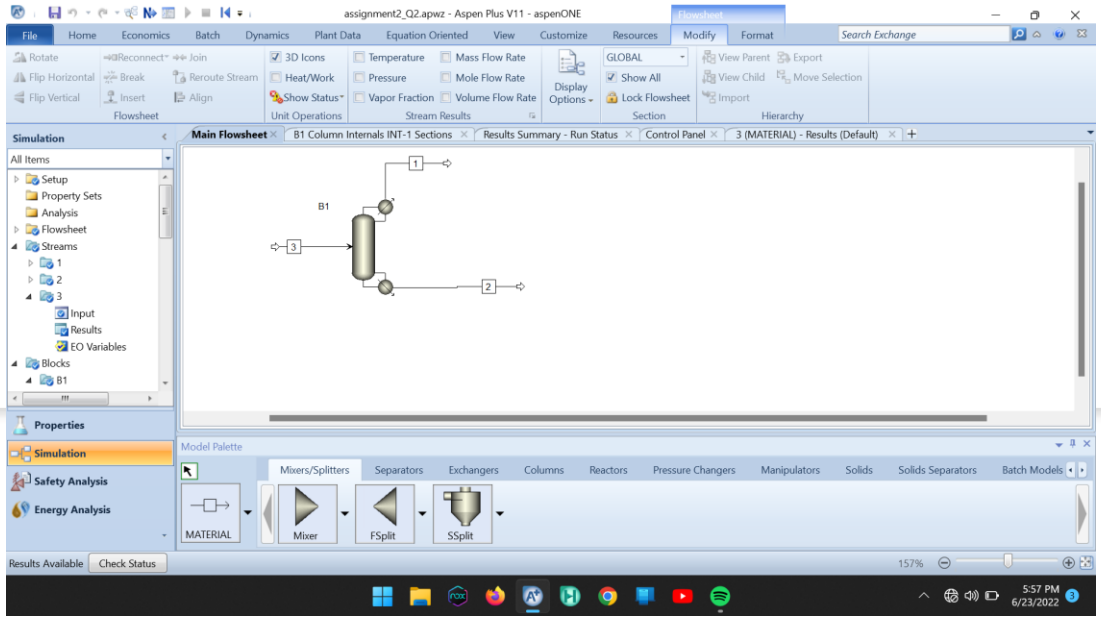
Q2).

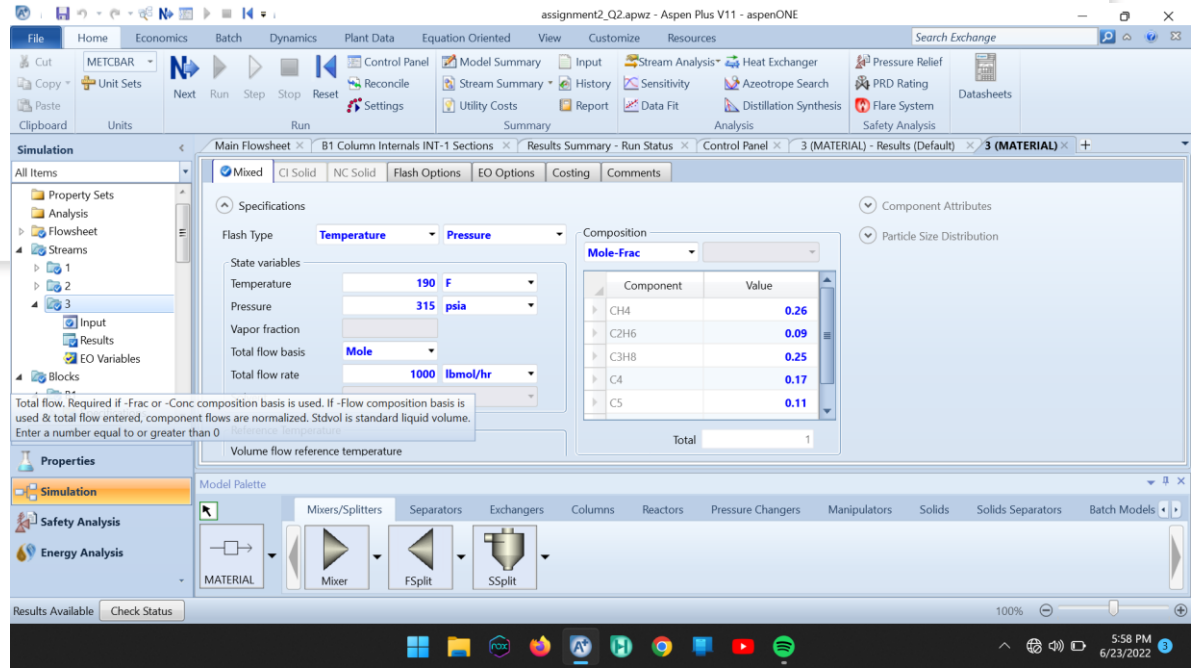
RadFrac demonstration

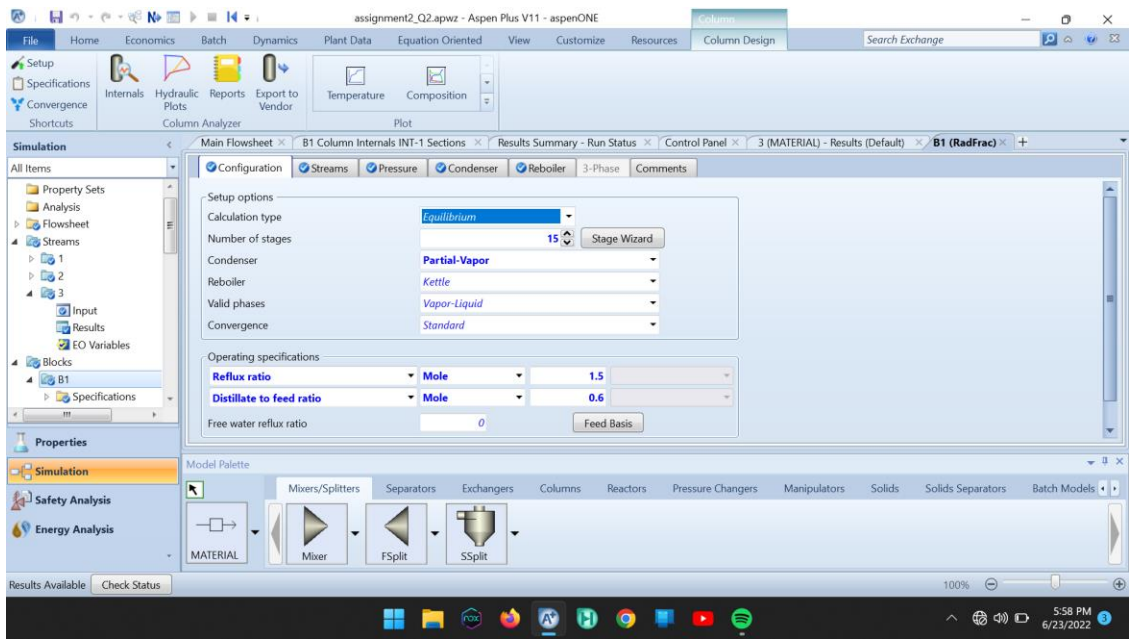


- RadFrac Specifications
- Partial condenser
- Kettle reboiler
- 15 stages
- R = 1.5
- Distillate to feed ratio = 0.6
- Column pressure = 315 psia
- Feed stage = 8

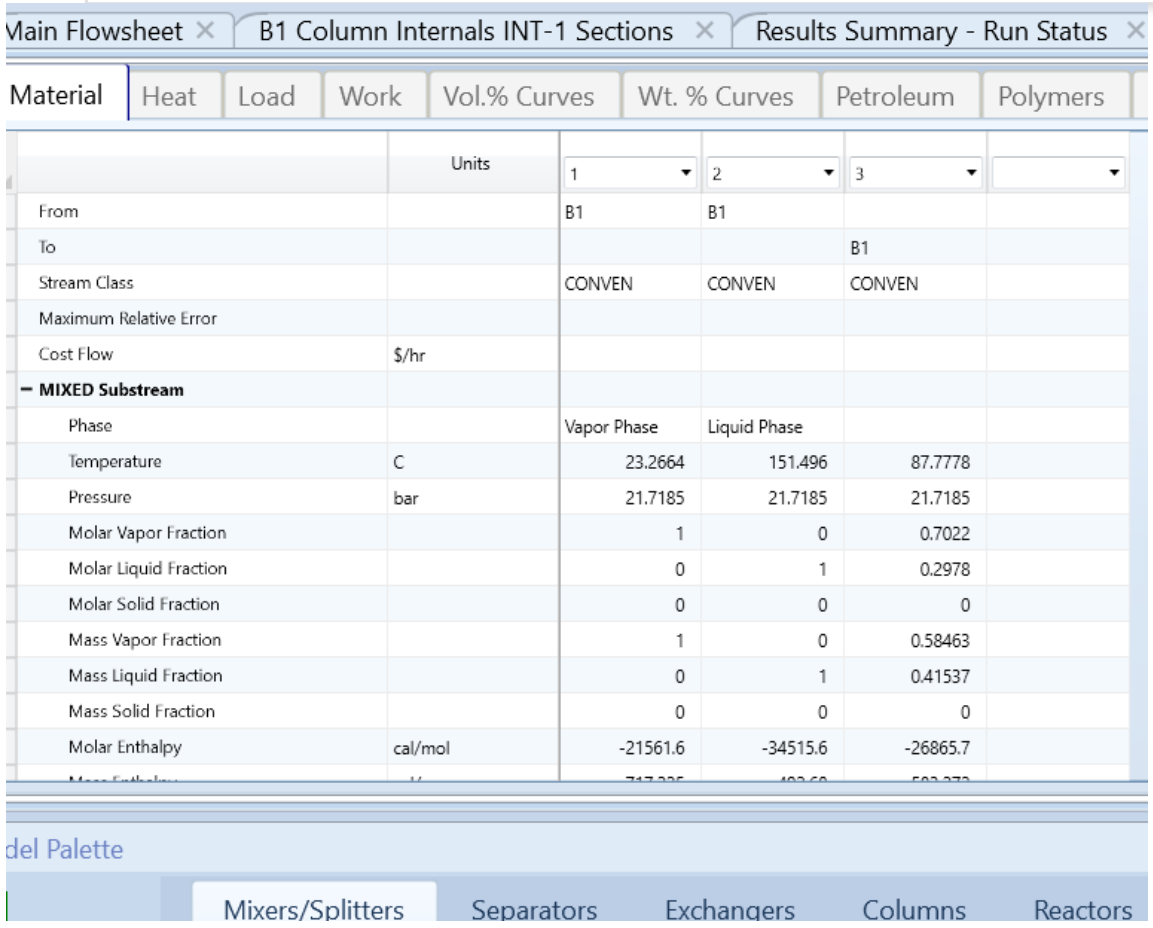
Use the RKS-BM Property method

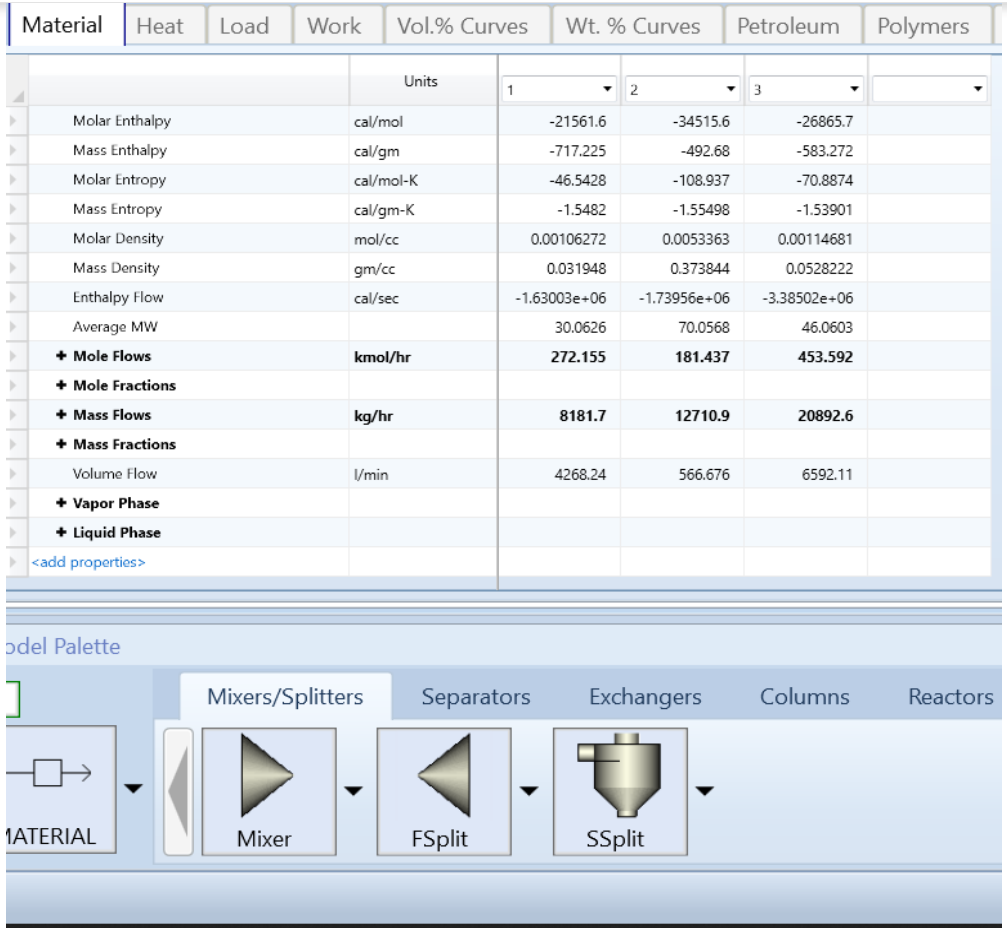

assignment2_Q2.apwz - Aspen Plus V11 - aspenONE
Main Flowsheet
B1 Column Internals INT-1 Sections
Results Summary - Run Status
Control Panel
3 (MATERIAL) - Results (Default)
B1
MATERIAL
Mixer
FSplit
SSplit
Results Available
Check Status
5:57 PM
6/23/2022


assignment2_Q2.apwz - Aspen Plus V11 - aspenONE
3 (MATERIAL)
Mixed
CI Solid
NC Solid
Flash Options
EO Options
Costing
Comments
Specifications
Flash Type
Temperature
Pressure
State variables
Temperature 190 F
Pressure 315 psia
Vapor fraction
Total flow basis Mole
Total flow rate 1000 lbmol/hr
Volume flow reference temperature
Composition
Mole-Frac
Component
Value
CH4 0.26
C2H6 0.09
C3H8 0.25
C4 0.17
C5 0.11
Total 1
Component Attributes
Particle Size Distribution
Total flow. Required if -Frac or -Conc composition basis is used. If -Flow composition basis is used & total flow entered, component flows are normalized. Stdvol is standard liquid volume. Enter a number equal to or greater than 0
MATERIAL
Mixer
FSplit
SSplit
Results Available
Check Status
5:58 PM
6/23/2022


assignment2_Q2.apwz - Aspen Plus V11 - aspenONE
Column Design
B1 (RadFrac)
Configuration
Streams
Pressure
Condenser
Reboiler
3-Phase
Comments
Setup options
Calculation type Equilibrium
Number of stages 15
Stage Wizard
Condenser Partial-Vapor
Reboiler Kettle
Valid phases Vapor-Liquid
Convergence Standard
Operating specifications
Reflux ratio Mole 1.5
Distillate to feed ratio Mole 0.6
Free water reflux ratio 0
Feed Basis
MATERIAL
Mixer
FSplit
SSplit
Results Available
Check Status
5:58 PM
6/23/2022

- Stream results:-





- Problem 3 :-

Q3).

2. **(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.

Assignment2_q3.apwz - Aspen Plus V11 - aspenONE

Flowsheet

File | Home | Economics | Batch | Dynamics | Plant Data | Equation Oriented | View | Customize | Resources | Modify | Format

Search Exchange

Rotate | Flip Horizontal | Flip Vertical | Reconnect | Break | Insert | Join | Reroute Stream | Align — Flowsheet

3D Icons | Heat/Work | Show Status — Unit Operations

Temperature | Pressure | Vapor Fraction | Mass Flow Rate | Mole Flow Rate | Volume Flow Rate — Stream Results

Display Options

GLOBAL | Show All | Lock Flowsheet — Section

View Parent | View Child | Import | Export | Move Selection — Hierarchy

Simulation

All Items

- Setup
- Property Sets
- Analysis
- Flowsheet
- Streams
- Blocks
  - B1
    - Input
    - Block Options
    - EO Modeling
    - Results
    - Stream Results
    - Summary
- Utilities

Properties

Simulation

Safety Analysis

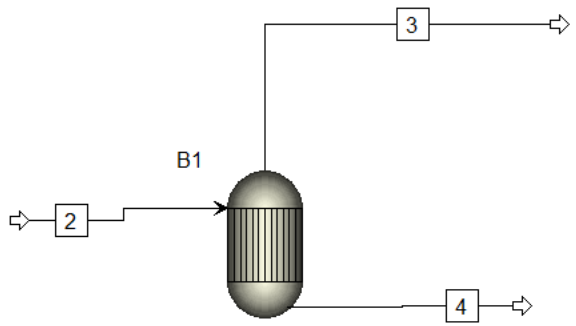
Energy Analysis

Capital: ____USD Utilities: ____USD/Year

Energy Savings: ____MW (____%)

Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet | B1 (REquil) - Stream Results (Boundary) | Setup | B1 (REquil) - Input | Control Panel | Utilities | Results Summary



Model Palette

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

MATERIAL | Mixer | FSplit | SSplit

Results Available (problem not yet run) | Check Status

167%

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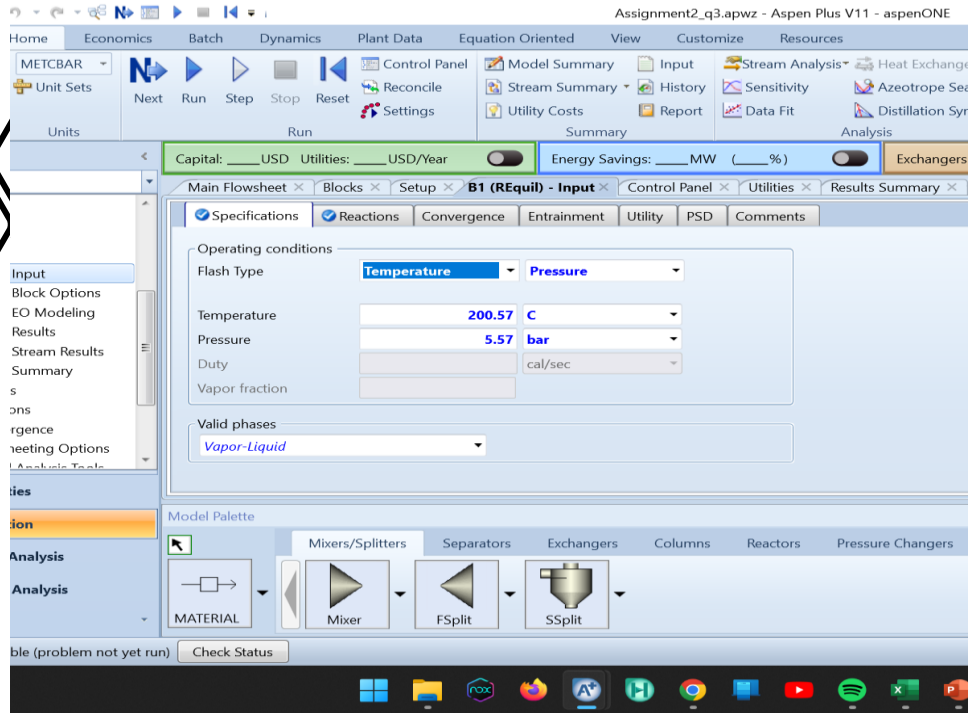
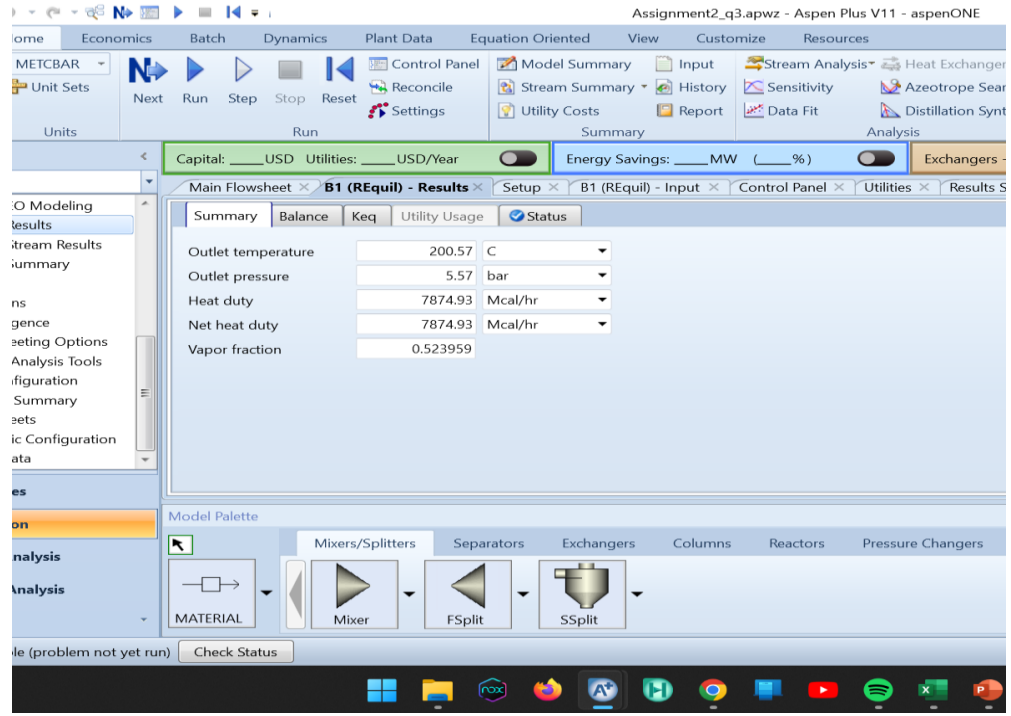
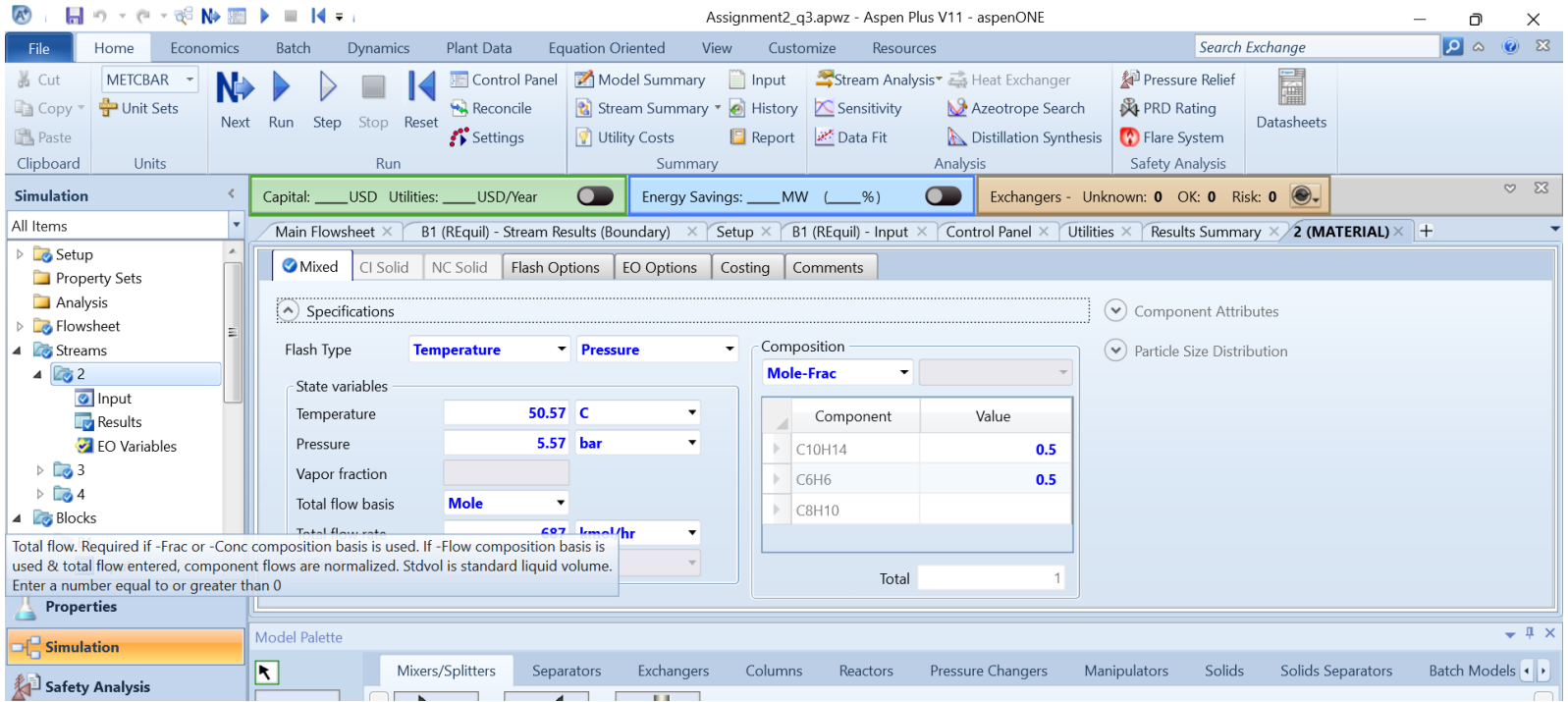

Assignment2_q3.apwz - Aspen Plus V11 - aspenONE
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Main Flowsheet
Blocks
Setup
B1 (REquil) - Input
Control Panel
Utilities
Results Summary
Specifications
Reactions
Convergence
Entrainment
Utility
PSD
Comments
Operating conditions
Flash Type
Temperature
Pressure
Temperature 200.57 C
Pressure 5.57 bar
Duty cal/sec
Vapor fraction
Valid phases
Vapor-Liquid
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
MATERIAL
Mixer
FSplit
SSplit
Check Status


Assignment2_q3.apwz - Aspen Plus V11 - aspenONE
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Main Flowsheet
B1 (REquil) - Results
Setup
B1 (REquil) - Input
Control Panel
Utilities
Summary
Balance
Keq
Utility Usage
Status
Outlet temperature 200.57 C
Outlet pressure 5.57 bar
Heat duty 7874.93 Mcal/hr
Net heat duty 7874.93 Mcal/hr
Vapor fraction 0.523959
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
MATERIAL
Mixer
FSplit
SSplit
Check Status


Assignment2_q3.apwz - Aspen Plus V11 - aspenONE
File
Home
Economics
Batch
Dynamics
Plant Data
Equation Oriented
View
Customize
Resources
Search Exchange
Cut
Copy
Paste
Clipboard
METCBAR
Unit Sets
Units
Next
Run
Step
Stop
Reset
Control Panel
Reconcile
Settings
Run
Model Summary
Stream Summary
Utility Costs
Input
History
Report
Summary
Stream Analysis
Sensitivity
Data Fit
Heat Exchanger
Azeotrope Search
Distillation Synthesis
Analysis
Pressure Relief
PRD Rating
Flare System
Safety Analysis
Datasheets
Simulation
All Items
Setup
Property Sets
Analysis
Flowsheet
Streams
2
Input
Results
EO Variables
3
4
Blocks
Properties
Simulation
Safety Analysis
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Exchangers - Unknown: 0 OK: 0 Risk: 0
Main Flowsheet
B1 (REquil) - Stream Results (Boundary)
Setup
B1 (REquil) - Input
Control Panel
Utilities
Results Summary
2 (MATERIAL)
Mixed
CI Solid
NC Solid
Flash Options
EO Options
Costing
Comments
Specifications
Component Attributes
Particle Size Distribution
Flash Type Temperature Pressure
State variables
Temperature 50.57 C
Pressure 5.57 bar
Vapor fraction
Total flow basis Mole
Total flow rate kmol/hr
Composition
Mole-Frac
Component Value
C10H14 0.5
C6H6 0.5
C8H10
Total 1
Total flow. Required if -Frac or -Conc composition basis is used & total flow entered, component flows are normalized. Stdvol is standard liquid volume.
Enter a number equal to or greater than 0
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
Batch Models

Stream results :-

	Units	2	3	4	
+ **Mole Flows**	**kmol/hr**	**687**	**359.96**	**327.04**	
+ **Mole Fractions**					
+ **Mass Flows**	**kg/hr**	**72937**	**34611.2**	**38325.8**	
+ **Mass Fractions**					
Volume Flow	l/min	1423.01	37874.8	901.371	
+ **Vapor Phase**					
+ **Liquid Phase**					
<add properties>					

Main Flowsheet | Blocks | Setup | **B1 (REquil) - Stream Results (Boundary)** | Control Panel | Utilities | Results Summary | 2 (M

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	2	3	4	
Description					
From			B1	B1	
To		B1			
Stream Class		CONVEN	CONVEN	CONVEN	
Maximum Relative Error					
Cost Flow	$/hr				
− **MIXED Substream**					
Phase		Liquid Phase	Vapor Phase	Liquid Phase	
Temperature	C	50.57	200.57	200.57	

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	2	3	4	
Molar Enthalpy	cal/mol	32488.8	39179.4	49204.2	
Mass Enthalpy	cal/gm	306.015	407.47	419.867	
Molar Entropy	cal/mol-K	-100.531	-52.2429	-95.7331	
Mass Entropy	cal/gm-K	-0.946912	-0.543332	-0.816905	
Molar Density	mol/cc	0.00804635	0.000158399	0.00604709	
Mass Density	gm/cc	0.85426	0.0152305	0.708658	
Enthalpy Flow	cal/sec	6.19995e+06	3.9175e+06	4.46993e+06	
Average MW		106.167	96.1529	117.19	
+ **Mole Flows**	kmol/hr	687	359.96	327.04	

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	2	3	4	
Phase		Liquid Phase	Vapor Phase	Liquid Phase	
Temperature	C	50.57	200.57	200.57	
Pressure	bar	5.57	5.57	5.57	
Molar Vapor Fraction		0	1	0	
Molar Liquid Fraction		1	0	1	
Molar Solid Fraction		0	0	0	
Mass Vapor Fraction		0	1	0	
Mass Liquid Fraction		1	0	1	
Mass Solid Fraction		0	0	0	

odel Palette

Mixers/Splitters | Separators | Exchangers | Columns | Reactors | Pressure Changers | Manipulators | Soli

- Net heat duty :- 7874.93 Mcal/hr
- vp :- 0.5292

- Thank you