

Chemical Engineering Department

B.M.S College of Engineering

(Autonomous Institute, Affiliated to VTU)



VII SEMESTER

**Subject Titled: Chemical Process Modeling and
Simulation**

Subject Code: 16CH7DCPMS

Lab Manual

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List of Experiments

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2.	Modeling of Mixer in series with Heater
3.	Modeling of Mixer in series with Flash separator
4.	Flash Separation operation
5.	Simulation of Distillation column
6.	Simulation of Refrigeration Cycle including compressor
7.	Simulation of Multi-component Absorption Column
8.	Model of the heater and reactor system
9.	Simulation of Conversion reactor
10.	Modelling and simulation of CSTR

Problem 1: Modeling of Mixer

Model a mixing process with two inlet streams named as feed 1 and feed 2 where, temperature is 40°C and Pressure is 4000 kPa for both the streams. The flow rate of the feed 1 is 1000kg/h and the flow rate of feed 2 is 20kg/h. The composition of the Feed 1 and Feed 2 is shown in table. Determine the overall flow rate and composition of the mixed stream. Use Peng-Robinson, SRK and NRTL fluid packages.

	Feed1	Feed2
Components	Mole %	Mole %
CO ₂	25%	10%
H ₂	75%	90%

Process Flow Diagrams:

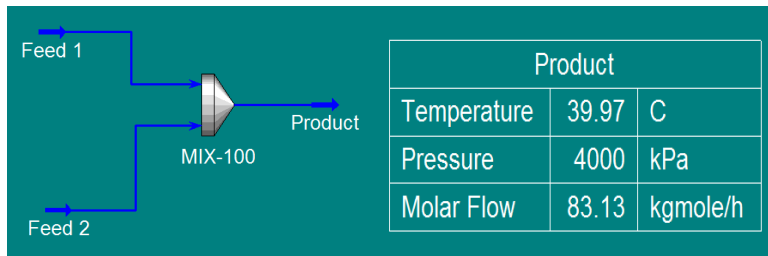


Fig 1.1 – Process diagram for mixing operation using Peng-Robinson fluid package

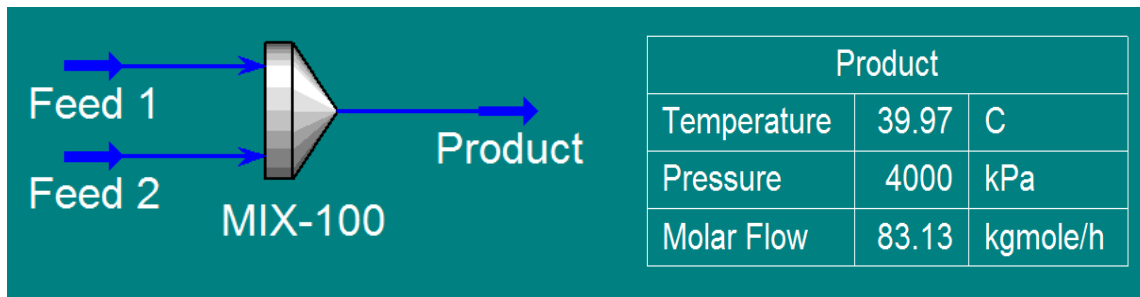


Fig 1.2 – Process diagram for mixing operation using SRK fluid package

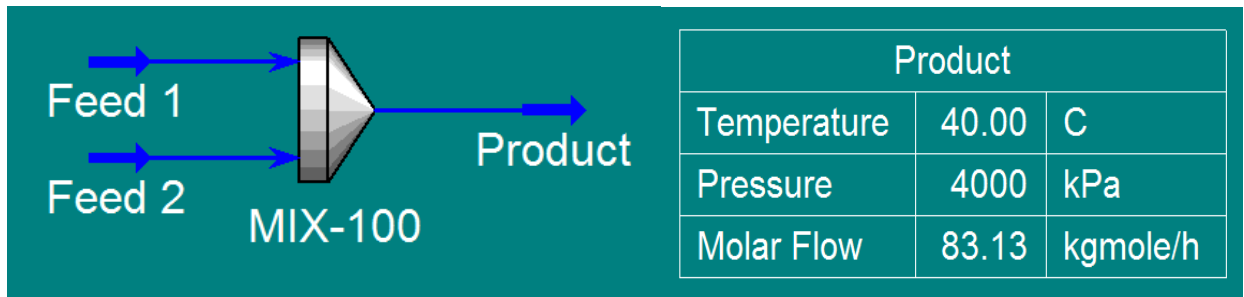


Fig 1.3 – Process diagram for mixing operation using NRTL fluid package

Procedure:

1. Open UNISIM software.
2. Select the required components from the component library and add pure components.
3. Select the required Fluid packages(SRK, Peng-Robinson and NRTL fluid packages)
4. Enter the simulation environment.
5. Select mixer, MIX-100 flow symbol from object palette.
6. Enter the required parameters for feed 1 and feed 2 as given in the problem statement.
7. Tabulate the mixer worksheet.

Table1.1: Worksheet for mixer model using SRK fluid package

Name of the Variables	Feed 1	Feed 2	Product
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table1.2: Worksheet for mixer model using Peng-Robinson fluid package

Name of the Variables	Feed 1	Feed 2	Product
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table1.3: Worksheet for mixer model using NRTL fluid package

Name of the Variables	Feed 1	Feed 2	Product
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

1.4 Result Table for all the fluid packages used

Fluid packages	Overall mass flow rate of product stream (kg/hr)	Components	Composition in product stream
SRK		Hydrogen	
		CO ₂	
Peng-Robinson		Hydrogen	
		CO ₂	
NRTL		Hydrogen	
		CO ₂	

Inference:

Problem 2: Modeling of Mixer in series with Heater

Simulate a mixer with heater model. The initial conditions two inlet streams are as follows, temperature is 40°C and Pressure is 4000 kPa. The flow rate of the CO₂ is 1000kg/h and the flow rate of H₂ is 20kg/h. The composition of the two feed streams is given in the table below, mixed stream from mixer is sent into the heater. Pressure drop in heater is 50 kPa, outlet stream of heater is 200 °C. Apply Peng Robinson Fluid package

- i. Determine the pressure of outlet stream and heater duty.
- ii. Simulate the developed model by varying the pressure drop conditions in the heater for
 - No Pressure drop
 - 20Kpa
 - 40Kpa
 - 80Kpa

	Feed1	Feed2
Components	Mole %	Mole %
CO ₂	25%	10%
H ₂	75%	90%

Process flow diagram:

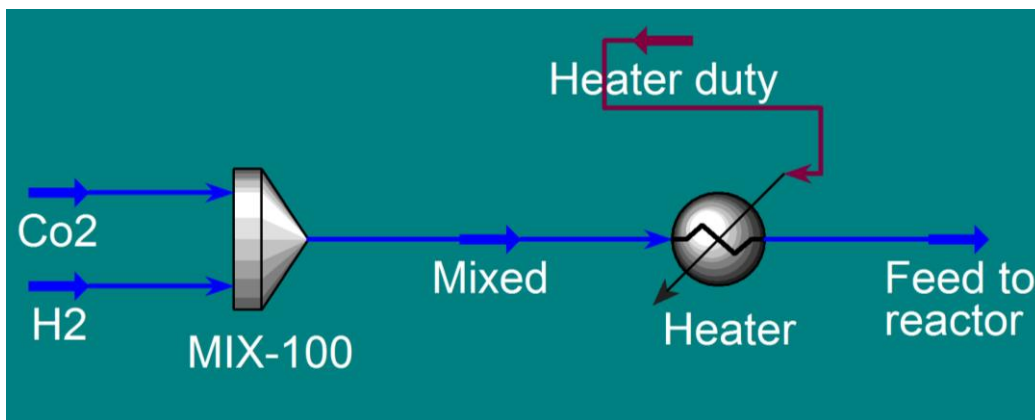


Fig 2.1: Process flow diagram

Procedure:

1. Open UNISIM software.
2. Select the components (Carbon dioxide and hydrogen) from the drop down menu
3. Click on fluid packages and choose Peng-Robinson and proceed to simulation environment.
4. Click on the mixer unit operation icon from the object pellet
5. Enter all the initial conditions of the feed streams
6. Click on worksheet and tabulate the outlet conditions of the mixed stream.
7. Select the heater from the object pellet and place it on the simulation environment.
8. Double click the heater and connect the mixed stream as heater input and define the outlet stream of the heater
9. Move to heater worksheet enter the temperature of the outlet stream in the worksheet and the pressure drop under parameters.
10. Tabulate the results and repeat Step 9, for different values of pressure drop.

Table 2.1: Worksheet for mixer model

Name of the Variables	Feed 1	Feed 2	Product
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table 2.2: Worksheet for heater model

Name of the Variables	Mixed	Feed to reactor	Heater Duty
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table 2.3: Result Table effect of pressure drop

Name of the Variables	For $\Delta P=50\text{kPa}$		For $\Delta P=0\text{kPa}$		For $\Delta P=20\text{kPa}$		For $\Delta P=40\text{kPa}$		For $\Delta P=80\text{kPa}$	
Mixed Stream Temperature (°C)										
Feed to reactor Stream Temperature (°C)										
Feed to reactor Stream Pressure (kPa)										
Overall Duty (kJ/h)										
Composition in Mixed stream	H ₂		H ₂		H ₂		H ₂		H ₂	
Composition in Feed to reactor Stream	CO ₂		CO ₂		CO ₂		CO ₂		CO ₂	

Inference:

Problem 3: Modeling of Mixer in series with Flash separator

Model a mixer, stream 1 enters at temperature -220°C and pressure of 101.325 kPa. Stream 2 enters at temperature -250°C and pressure of 101.325 kPa. Simulate the mixer unit and separate the vapour and liquid phase streams using NRTL fluid package. The inlet streams composition is indicated in the table below.

- Estimate the composition of the mixed stream and its phase behavior.
- Estimate the mass flow rates of vapour and liquid phase stream in flash separator
- Estimate the composition of the vapour and liquid phase in flash separator

	Feed1	Feed2
Components	Mole %	Mole %
CO ₂	25%	10%
H ₂	75%	90%

Process flow diagram:

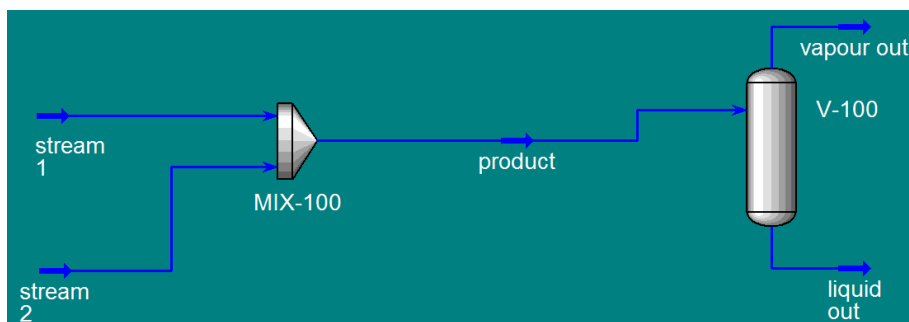


Fig 3.1: Process Flow Diagram of the mixer with Flash operation

Procedure:

- Open UNISIM software.
- Select the required components (H₂ and CO₂) and add them.
- Add the required fluid package (NRTL).
- Now enter to simulation environment.
- Select mixer operation from the object palette.
- Name the feed streams as stream 1 and stream 2 and the outlet stream as product.
- Enter the required parameters as specified in the problem.
- Add a flash/separator and double click on it.
- Name the feed stream and product streams, connect the product stream from mixer unit as feed stream for flash operation
- Note down the composition of the final stream from the flash.

Table 3.1: Worksheet for mixer model

Name of the Variables	Feed 1	Feed 2	Product
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table 3.2: Worksheet for flash separator

Name of the Variables	Product	Liquid Out	Vapour out
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table 3.3: Result Table of Simulation

Material streams	Components	Composition in product stream
Product Stream	H ₂	
	CO ₂	
Liquid Out	H ₂	
	CO ₂	
Vapour out	H ₂	
	CO ₂	

Inference:

Problem 4: Flash Separation operation

100kmol/h feed consisting of 50 mole % of ethane and 50 mole % of water, enters a flash chamber at 100kPa and flow rate 100kmol/h. Applying the suitable property method, compute the Composition of the exit streams, Bubble Point and Dew Point.

Process flow diagram:

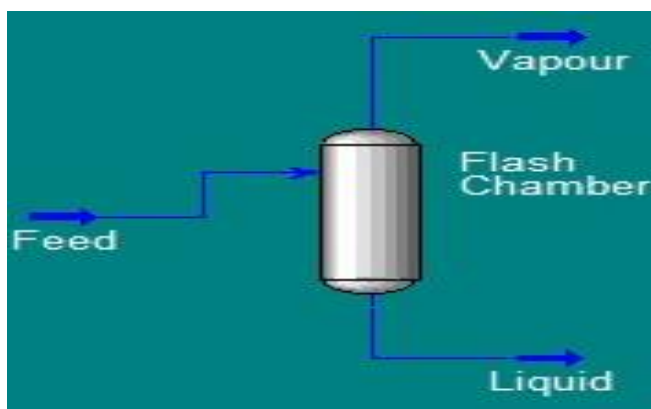


Fig - 4.1: Process Flow Diagram of the flash operation

Procedure:

1. Open UNISIM software.
2. Select the required components (Ethanol and water) and add them.
3. Select and add the required fluid package (NRTL).
4. Enter into the simulation environment.
5. Select the flash operation symbol from the object palette.
6. Define inlet stream as feed, product streams as liquid and vapor outlet streams.
7. Enter the initial feed conditions in the worksheet of the flash separator.
8. Enter in to the composition tab in the worksheet of the feed stream.
9. Under conditions, set vapor of feed as 1 as everything is in vapor state and the dew point is obtained.
10. To obtain the bubble point set vapor of feed as 0.
11. Note down the composition of the product stream.
12. The procedure is repeated for SRK and Peng-Robinson fluid package.

Table - 4.1: Overall Worksheet of the flash operation at dew point

Name of the Variables	Feed	Liquid Out	Vapour out
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table - 4.2: Composition values at dew point

Material streams	Components	Composition in product stream
Feed Stream	Ethanol	
	Water	
Liquid Out	Ethanol	
	Water	
Vapour out	Ethanol	
	Water	

Table - 4.3: Overall Worksheet of the flash operation at bubble point

Name of the Variables	Feed	Liquid Out	Vapour out
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table - 4.4: Composition values at dew point

Material streams	Components	Composition in product stream
Feed Stream	Ethanol	
	Water	
Liquid Out	Ethanol	
	Water	
Vapour out	Ethanol	
	Water	

Table - 4.5: Result Table

Temperatures	Components	Streams	Compositions
Bubble Temp:	Ethanol	Liquid outlet	
	Water		
Dew Point Temp:	Ethanol	Vapour outlet	
	Water		

Inference:

PROBLEM 5: Simulation of Distillation column

A continuous fractionating column having 17 stages with total condenser and re-boiler is to be designed to separate a feed flowing at a rate of 2752.2 kmol/hr. The feed is a mixture of 28.19 % methanol, 46.26% n-butane and 25.55 % 1-butene on molar basis. A reflux ratio of 10 mol to 1 mol of product is to be used. The feed enters at bubble point and pressure of 1172 kPa in the 10th stage. Overhead product flows out at a rate of 2043.0 kmol/ hr. The pressure at condenser and re-boiler are 1115 kPa and 1216 kPa respectively. Simulate using UNISIM design suite and estimate the following

- Conditions and properties of feed, distillate and bottom streams
- Composition of distillate and bottom products
- The temperature variation with respective tray position.
- The liquid rate and vapor rate profiles
- Composition profiles of all the components
- Heat duties required for the condenser and re-boiler
- Temperature of condenser and re-boiler.

Process flow diagram:

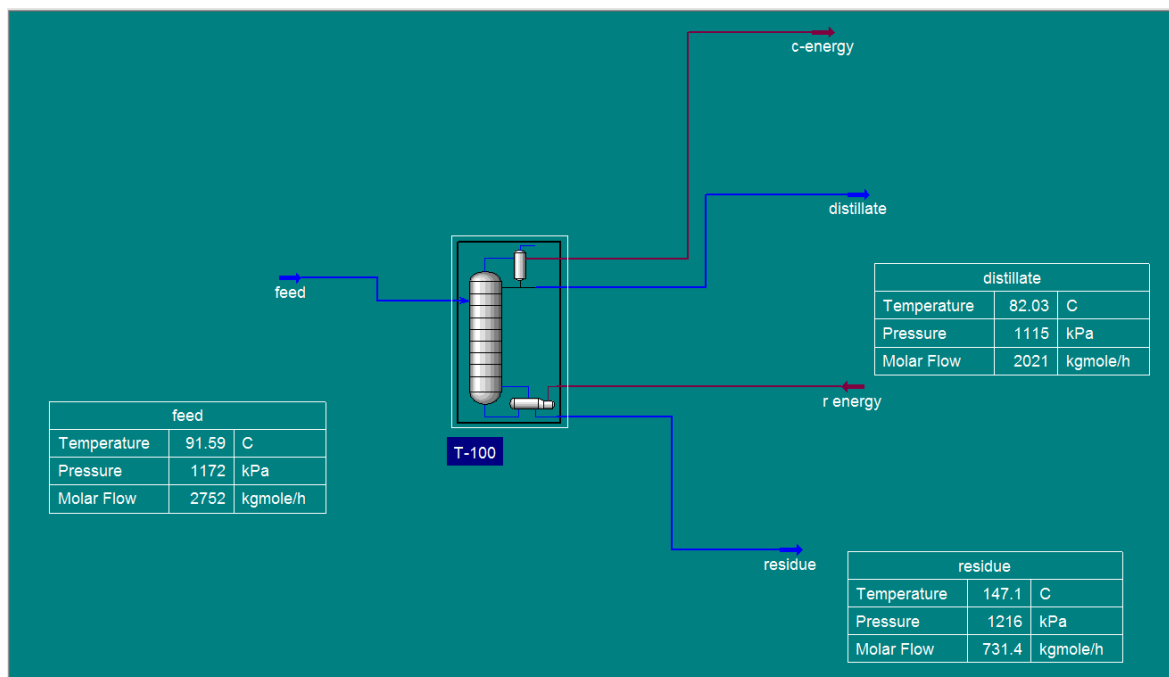


Fig 5.1 – Process flow diagram for distillation column

Procedure:

1. Get started with the UNISIM Design Software
2. Add the components involved in the process. Here methanol, n-butane and 1-butene were added
3. Select the suitable fluid package to analyze the properties of the system. Peng-Robinson package was selected.
4. Enter the simulation environment.
5. Select the distillation column from the palette and the inlets and outlets streams are defined
6. Enter the initial feed conditions (minimum 3 conditions) namely the vapor fraction, molar flow and the pressure values were entered.
7. Compositions of the inlet feed was also entered as given in the problem statement
8. Reflux Ratio and the other required parameters are entered
9. We check for the temperature plot and try to change the number of plates for optimization

Table – 5.1: Condition table for feed stream

Name of the Variables	Feed	Liquid Phase	Vapour Phase
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table – 5.2: Condition table for Distillate and Residue streams

Name of the Variables	Distillate	Liquid Phase	Residue	Liquid Phase
Vapour				
Temperature (°C)				
Pressure (kPa)				
Molar flow rate (kmol/h)				
Mass flow rate (kg/h)				
Std. ideal liquid Vol flow (m ³ /h)				
Molar Enthalpy (KJ/kgmol. °C)				
Molar Entropy (KJ/kgmol. °C)				
Heat Flow (KJ/h)				

Table – 5.3: Composition table for Distillate and Residue streams

Material Streams	Components	Composition in mole fractions
Distillate	Methanol	
	n-Butane	
	1-Butene	
Residue	Methanol	
	n-Butane	
	1-Butene	

Table – 5.4: Heat duties for condenser and residue streams

Name of the stream	Heat Duties Required (kJ/hr)	Temperature (°C)
Condenser		
Reboiler		

Inference:

Problem 6: Simulation of Refrigeration Cycle including compressor

The Refrigerator R-134a is used as a working fluid. The mass flow through each component is 0.1kg/s and the power input to the compressor is 5kw. The heat lost to the compressor is 0.21kw. The following state data given $P_1= 100\text{kpa}$, $T_1=-20^\circ\text{C}$, $P_2=800\text{kpa}$, $x_3=0.0$ and $T_4=-25^\circ\text{C}$. Simulate the given refrigeration cycle using Unisim design tool for Peng Robinson and SRK fluid packages.

Determine the

- i. Quality of the evaporator inlet
- ii. Rate of heat transfer to the evaporator
- iii. Mass flow of cold water in the condenser and evaporator.
- iv. Pressure and temperature in all the four states.

Data Given: Temperature difference in condenser is from 10°C to 15°C and in the evaporator is 85°C to 45°C .

Process flow diagram:

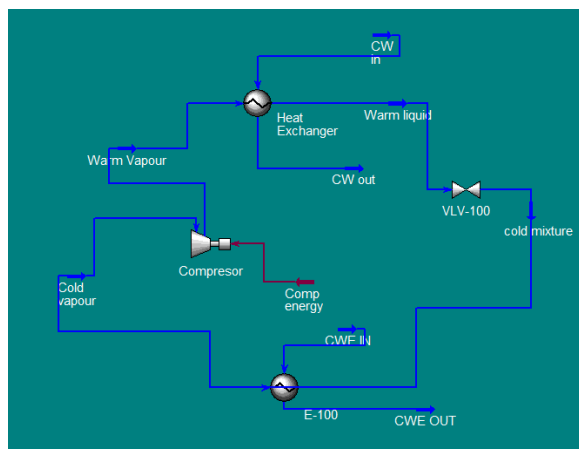


Fig. 8.1: Process flow diagram for refrigeration cycle

Procedure:

1. Open new simulation File R443, select a suitable fluid package (Peng Robinson and SRK models) add the components required.
2. Enter the simulation environment and add the compressor operation, define the streams and conditions provided.
3. Enter all the details given in the problem.

4. Select the condenser from the object palette and connect warm vapor as tube side inlet and cold water as shell side inlet.
5. Enter the composition of cold water inlet
6. Connect the cold liquid outlet of condenser as inlet to expansion valve.
7. Select evaporator from object palette and connect cold mixture which is outlet of expansion valve as tube side inlet to the evaporator.
8. Shell side inlet as cold water and enter its composition
9. Note down all the results obtained for each unit operations

Table – 6.1: Condition table for Compressor operation

Name of the Variables	Cold vapour	Warm Vapour
Vapour		
Temperature (°C)		
Pressure (kPa)		
Molar flow rate (kmol/h)		
Mass flow rate (kg/h)		
Std. ideal liquid Vol flow (m ³ /h)		
Molar Enthalpy (KJ/kgmol. °C)		
Molar Entropy (KJ/kgmol. °C)		
Heat Flow (KJ/h)		

Table – 6.2: Condition table for Condenser operation

Name of the Variables	Warm Vapour	Cold Liquid	Cold Water in	Cold Water out
Vapour				
Temperature (°C)				
Pressure (kPa)				
Molar flow rate (kmol/h)				
Mass flow rate (kg/h)				
Std. ideal liquid Vol flow (m ³ /h)				
Molar Enthalpy (KJ/kgmol. °C)				
Molar Entropy (KJ/kgmol. °C)				
Heat Flow (KJ/h)				

Table – 6.3: Composition table at condenser operation

Material Streams	Components	Composition in mole fractions
Warm Vapour	R-134a	
	Water	
Cold Liquid	R-134a	
	Water	
Cold Water in	R-134a	

	Water	
Cold Water out	R-134a	
	Water	

Table – 6.4: Condition table for Expansion Value

Name of the Variables	Cold Liquid	Cold Mixture
Vapour		
Temperature (°C)		
Pressure (kPa)		
Molar flow rate (kmol/h)		
Mass flow rate (kg/h)		
Std. ideal liquid Vol flow (m ³ /h)		
Molar Enthalpy (KJ/kgmol. °C)		
Molar Entropy (KJ/kgmol. °C)		
Heat Flow (KJ/h)		

Table – 6.5: Condition table for Evaporator operation

Name of the Variables	Cold Mixture	Cold Vapour	Water in	Water out
Vapour				
Temperature (°C)				
Pressure (kPa)				
Molar flow rate (kmol/h)				
Mass flow rate (kg/h)				
Std. ideal liquid Vol flow (m ³ /h)				
Molar Enthalpy (KJ/kgmol. °C)				
Molar Entropy (KJ/kgmol. °C)				
Heat Flow (KJ/h)				

Table – 6.6: Composition table at Evaporator operation

Material Streams	Components	Composition in mole fractions
Cold Mixture	R-134a	
	Water	
Cold Vapour	R-134a	
	Water	
Water in	R-134a	
	Water	
Water out	R-134a	
	Water	

Inference:

Problem 7: Simulation of Multi-component Absorption Column

An Absorber contains 20 trays and operates at 60psia charges a wet gas of composition given in Table 1 at 90°F. The lean oil can be assumed to have the composition properties of normal ctane, and at present has a maximum circulation rate of 0.905 times the wet gas rate. A modification in the design of the column increased the oil circulation rate to 1.104 times that of wet gas rate. At this expected rate, the lean oil will enter the column at temperature of 90°F and contains 2 mol% of n-butane and 5 mol% of n-pentane.

- Estimate the recovery of each of the gas components at the new oil rate.
- Determine the corresponding product rate and composition
- Obtain the Variation of temperature, pressure and composition with respect to tray position.

Note: Assume that the absorber stage efficiency is 20% for all the components.

Components	Mole Fractions
C1: Methane	0.285
C2: Ethane	0.158
C3: Propane	0.240
n-C4: Butane	0.169
n-C5: Pentane	0.148
Total	1.00

Process flow diagram:

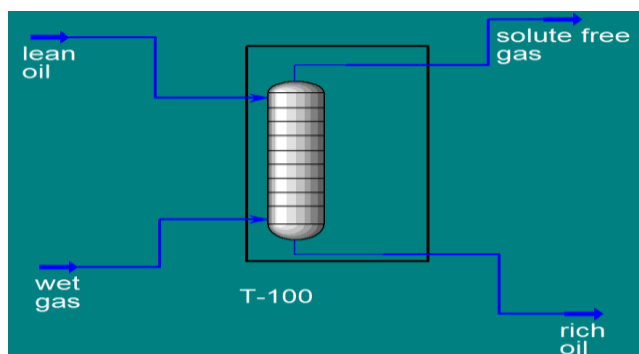


Fig. 7.1: Schematic representation of an Absorber Column

Procedure:

- Open new simulation File R443, select a suitable fluid package: Peng Robinson and the components required.
- Enter the simulation environment and select the absorption column from the object palette.

3. Name the streams and enter the no of stages required as 4 because there are 20 stages each of 20% efficiency as given in the question
4. Consider lean oil in the top stage inlet, Wet gas in the bottom stage inlet, Solute free gas is in the overhead vapor outlet and rich oil in the Bottom liquid outlet.
5. Enter the top stage and bottom stage pressure values.
6. Enter all the details for wet gas and lean oil stream given in the problem.
7. Run the Simulation after entering the stream values.

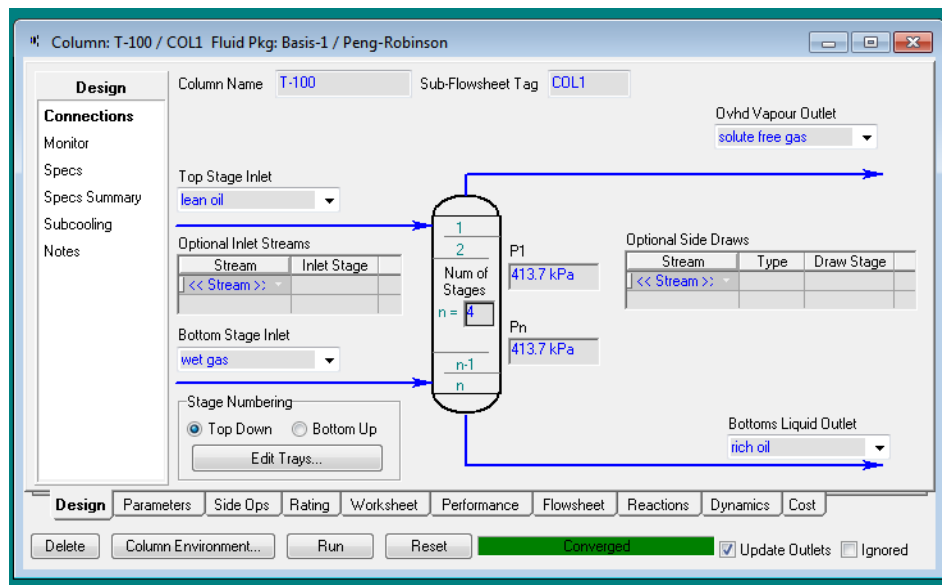


Fig 7.2: Design model of the Absorption column

Note: The top down approach has been used for the above question.

Table – 7.1: Condition table for Absorption column

Name of the Variables	Lean oil	Wet gas	Rich oil	Solute free gas
Vapour				
Temperature (°C)				
Pressure (kPa)				
Molar flow rate (kmol/h)				
Mass flow rate (kg/h)				
Std. ideal liquid Vol flow (m ³ /h)				
Molar Enthalpy (KJ/kgmol. °C)				
Molar Entropy (KJ/kgmol. °C)				
Heat Flow (KJ/h)				

Table – 7.2: Composition table at Absorption operation

Components	Lean oil	Wet gas	Rich oil	Solute free gas
C1: Methane				
C2: Ethane				
C3: Propane				
n-C4: Butane				
n-C5: Pentane				
n-C8:Octane				

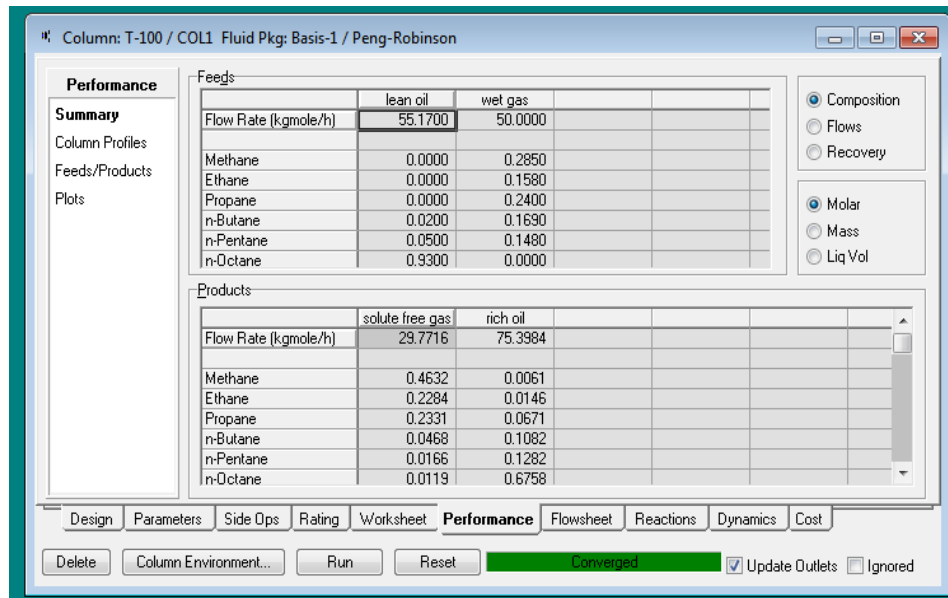
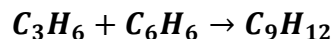


Fig 7.3: Absorption column performance summary table

Inference:

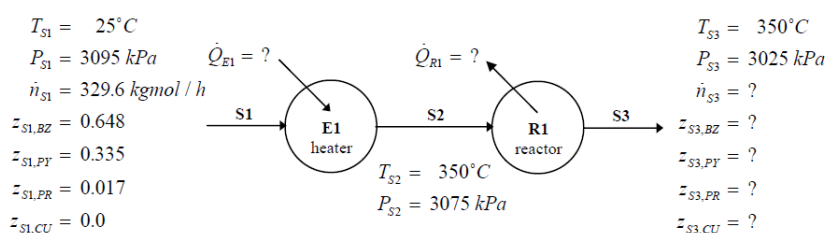
Problem 8: Model of the heater and reactor system

Model the conversion reactor using *UniSim* for converting propene and benzene to cumene under isothermal conditions, the reaction is vapour- phase reaction occurs as follows



The conceptual model of the reactor is given below in Fig 8.1. The molar conversion of the reactor is 83% for given catalyst.

- Determine the duty in kJ/h required to operate the isothermal reactor R1.
- How much heat is drawn from the exothermic reaction so that inlet and outlet streams of the reactor are at same temperature?



Process flow diagram:

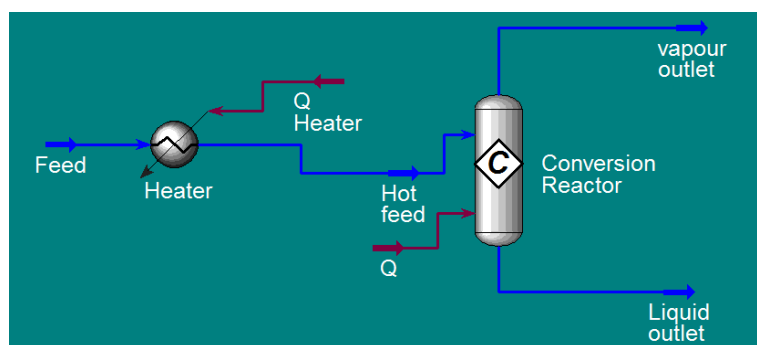


Fig 8.1: Conceptual model of the heater and reactor system

Procedure:

- Open new simulation File, select a suitable fluid package and the components required.
- Define the Reaction given in the reaction tab as conversion reaction and attach to the selected Fluid package
- Enter the simulation environment and select the Heater unit from the object palette.
- Name the material streams and Energy stream required
- Enter the Feed stream conditions and other conditions specified in the problem.

6. Select the Conversion reactor, define the streams and as shown in the process flow diagram
7. Tabulate the results obtained.

Table –8.1: Condition table for heater

Name of the Variables	Feed	Hot Feed	Q-heater
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table –8.2: Condition table for Conversion Reactor

Name of the Variables	Hot Feed	Liquid Outlet	Vapour Outlet
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table – 8.3: Composition table for Conversion Reactor

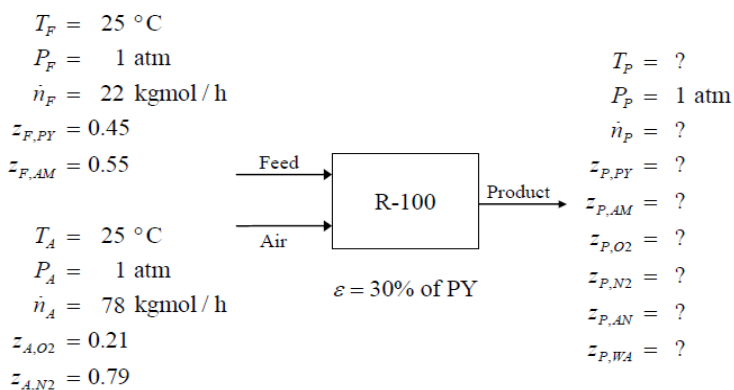
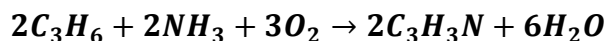
Components	Hot Feed	Liquid Outlet	Vapour Outlet
Propene			
Benzene			
Cumene			
Propane			

Inference:

Problem 9: Simulation of Conversion reactor

Let 45 mole% propylene and 55 mole % ammonia stream at 25°C and 1 atm are fed to the conversion reactor. The oxygen is fed to the reactor through the air stream at 25°C and 1 atm. The flow rate of the feed stream is 22kgmol/h, and the flow rate of the air stream is 78kgmol/h. Assume an adiabatic reactor with no pressure drop. Model and simulate the reactor to estimate the temperature & the dew point of the product stream from the reactor in Degree Celsius for 30% conversion of Propylene to Acrylonitrile. The conceptual model of the reactor is given below in Fig 3.2.

The reaction is given below



Process flow diagram:

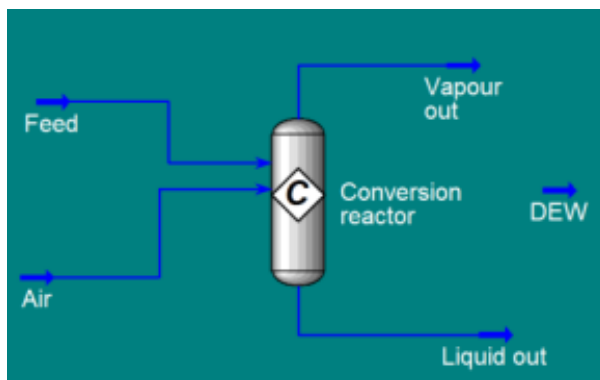


Fig 9.1: Conceptual model of the reactor

Procedure:

1. Open new simulation File, select a suitable fluid package and the components required.
2. Define the Reaction given in the reaction tab as conversion reaction and attach to the selected Fluid package

3. Enter the simulation environment and select the Conversion reactor, define the streams and as shown in the process flow diagram
4. Enter the Feed and Air streams conditions as specified in the problem.
5. Tabulate the results obtained for Bubble point and Dew point.

Table –9.1: Condition table for Conversion Reactor

Name of the Variables	Feed	Air	Liquid Outlet	Vapour Outlet
Vapour				
Temperature (°C)				
Pressure (kPa)				
Molar flow rate (kmol/h)				
Mass flow rate (kg/h)				
Std. ideal liquid Vol flow (m ³ /h)				
Molar Enthalpy (KJ/kgmol. °C)				
Molar Entropy (KJ/kgmol. °C)				
Heat Flow (KJ/h)				

Table – 9.2: Composition table for Conversion Reactor

Components	Feed	Air	Liquid Outlet	Vapour Outlet
Ammonia				
Nitrogen				
Oxygen				
Acrylonitril				
Water				

Result Table	
Product Out let temperature	
Dew point of product stream	

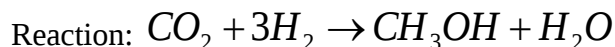
Inference:

Problem 10: Modeling and simulation of CSTR

Model a Continuous Stirred Tank Reactor (CSTR) with inlet stream named as Feed to Reactor is completely in vapour phase. The temperature of the reactor outlet is required to be 200°C. The liquid outlet stream named 'Dummy Liquid'. The feed stream flow rate 2500kg/h and the composition of the feed stream are given in the table below.

	Feed to reactor
Components	Mole Fraction
CO ₂	0.15%
H ₂	0.85%

- Determine the composition of product streams from the reactor by simulating using Unisim tool
- Optimize the size of the CSTR reactor for the given condition and interpret the results



Data: Pre-exponential Factor $A = 1.04 \times 10^{22}$; Activation Energy $E = 1.7 \times 10^5$ kJ.

Process flow diagram:

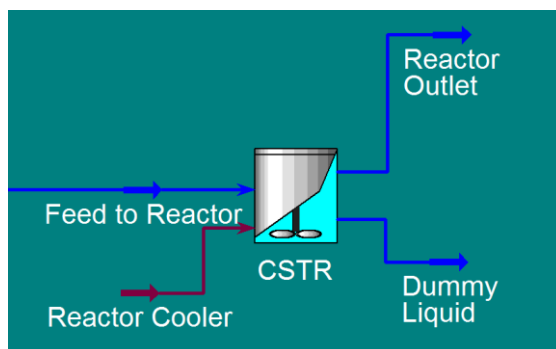


Fig 10.1: Conceptual model of the reactor

Procedure:

1. Open new simulation File, select a suitable fluid package and the components required.
2. Define the Reaction given in the reaction tab as conversion reaction and attach to the selected Fluid package
3. Enter the simulation environment and select the Conversion reactor unit from the object palette.
4. Name the material streams and Energy stream required as shown in the process flow diagram
5. Enter the Feed stream conditions and other conditions specified in the problem.
6. Tabulate the results obtained.

Table –10.1: Condition table for CSTR

Name of the Variables	Feed to reactor	Dummy Liquid	Reactor Outlet	Reactor cooler
Vapour				
Temperature (°C)				
Pressure (kPa)				
Molar flow rate (kmol/h)				
Mass flow rate (kg/h)				
Std. ideal liquid Vol flow (m ³ /h)				
Molar Enthalpy (KJ/kgmol. °C)				
Molar Entropy (KJ/kgmol. °C)				
Heat Flow (KJ/h)				

Table – 10.2: Composition table for Conversion Reactor

Components	Feed to reactor	Dummy Liquid	Reactor Outlet	Reactor cooler
CO ₂				
Hydrogen				
Methanol				
Water				

Inference: