

B.M.S. College of Engineering

Autonomous Institute, Affiliated to VTU

BENGALURU

DEPARTMENT OF CHEMICAL ENGINEERING



VI SEMESTER

Process Modeling and Simulation

22CH6PCPMS

LABORATORY MANUAL

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USN:

List of Experiments

S No	Experimental Title	Date of the Experiment	Marks Obtained	Sign of the faculty
1.	Simulation of flash drum for binary mixture			
2.	Simulation of distillation column			
3.	Simulation of absorption column			
4.	Simulation of heat exchanger			
5.	Simulation of two stage compression system			
6.	Simulation of refrigeration gas plant			
7.	Simulation of conversion reactor			
8.	Simulation of equilibrium reactor			
9.	Simulation of CSTR			
10.	Simulation of plug flow reactor			

Experiment No 1

Simulation of Flash Drum for Binary Mixture

Problem Statement: 100 kmol/h feed is a mixture of water and ethane. The composition of both water and ethane in feed stream are 50 Mole % each. Enters a flash chamber at 100 kPa and flow rate 100 kmol/h. Applying the suitable property method (any three fluid package), compute the composition of the exit streams, bubble point and dew point of the feed stream.

Process flow diagram:

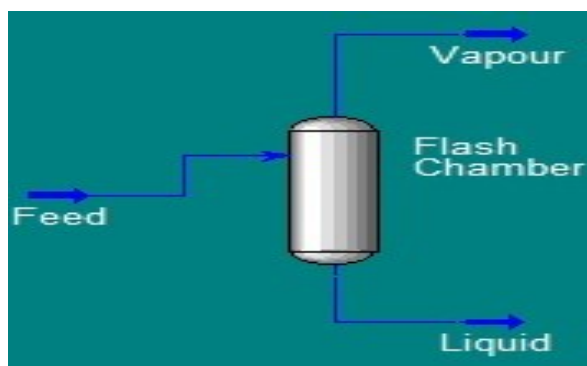


Fig - 1.1: Process Flow Diagram of the flash operation

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 into the composition tab in the worksheet of the feed stream.
9. Under conditions, set vapor fraction of feed the as 1 as everything is in vapor state and the dew point is obtained.
10. To obtain the bubble point set vapor fraction of the 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 - 1.1: 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 - 1.2: 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 - 1.3: 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 - 1.4: 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 - 1.5: Result Table

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

Inference:

Experiment No 2

Simulation of Distillation column

Problem Statement: A continuous fractionating column has 17 stages with total condenser and re-boiler. The column 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 and change Composition profiles of all the components with respective tray position.
- The liquid rate and vapor rate profiles.
- Heat duties required for the condenser and re-boiler.
- Temperature of condenser and re-boiler.

Process flow diagram:

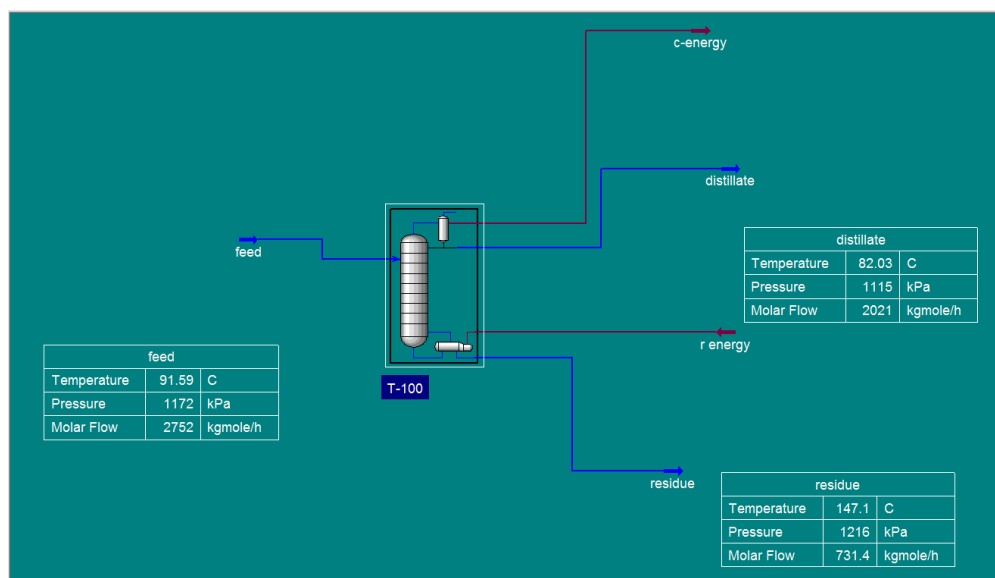


Fig 2.1 – Process flow diagram for distillation column

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. Run the simulation after entering the stream values.

Table – 2.1: 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 – 2.2: 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 – 2.3: 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 – 2.4: Heat duties for condenser and residue streams

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

Inference:

Experiment No 3

Simulation of absorption column

Problem Statement: 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:

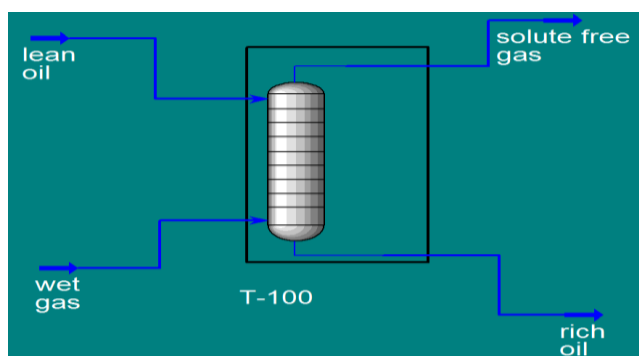


Fig. 3.1: Schematic representation of an Absorber Column

Procedure:

1. Get started with the UNISIM Design Software, select the components required, and select a suitable fluid package: Peng Robinson.
2. Enter the simulation environment and select the absorption column from the object palette.
3. Name the streams and enter the number 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.

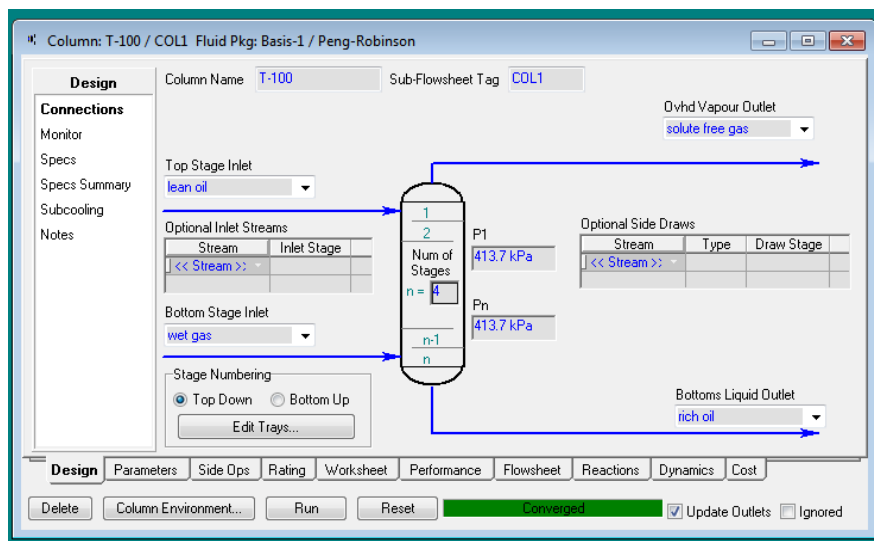


Fig 3.2: Design model of the Absorption column

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

Table – 3.1: 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 – 3.2: 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				

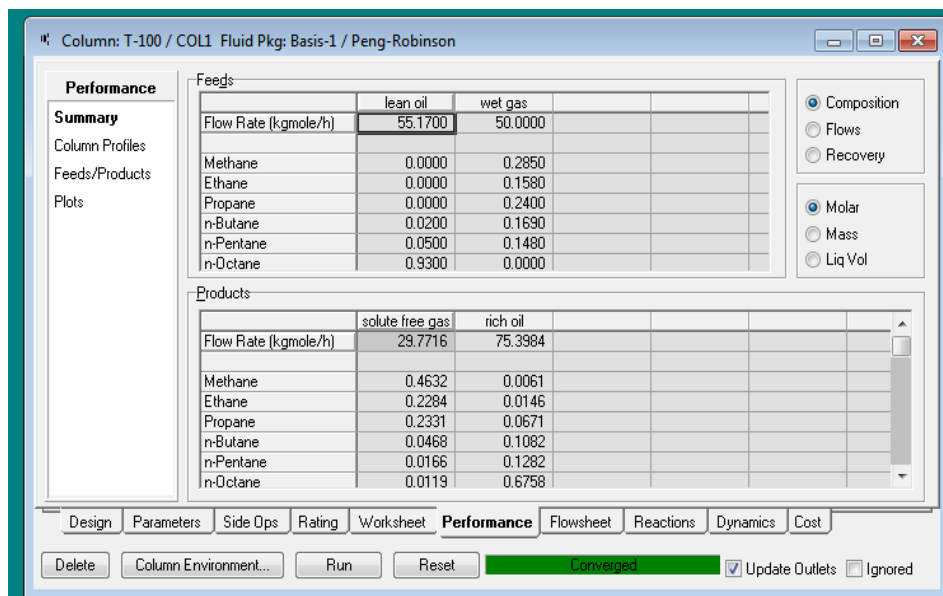


Fig 3.3: Absorption column performance summary table

Inference:

Experiment No 4

Simulation of heat exchanger

Problem Statement: Simulate an air-cooled shell and tube heat exchanger using UNSIM software. Initially 2000 kg/h of pure water is pumped from a storage tank into the heater. The water in the storage tank is at 25 °C and 1 bar pressure. The pressure of the water increases as it is pumped into the heater. The increase in pressure is around 3 bar. The water is heated in the heater, the raise in temperature in the heater is 85 °C. The hot water is sent into the heat exchanger in the tube side and the air enters through the shell side. The air leaves the heat exchanger at a temperature around 40 °C. The air flow rate into the heat exchanger is 4000 kg/h and at 1 bar pressure.

- Tabulate the condition table for all unit operations.
- Plot the profile for change in overall heat transfer coefficient, heat flow, and pressure with respect to temperature for both tube side and shell side.

Process flow diagram:

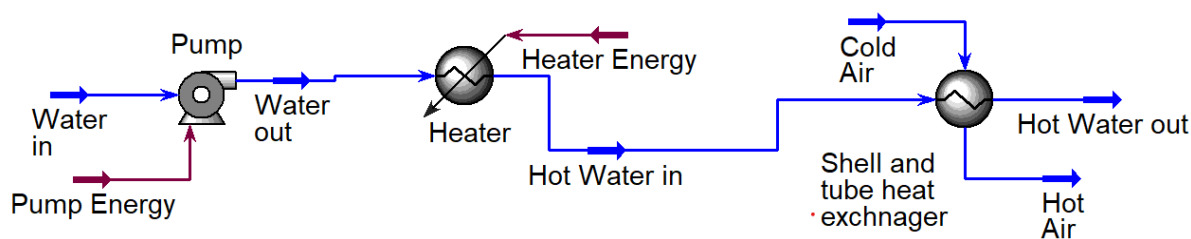
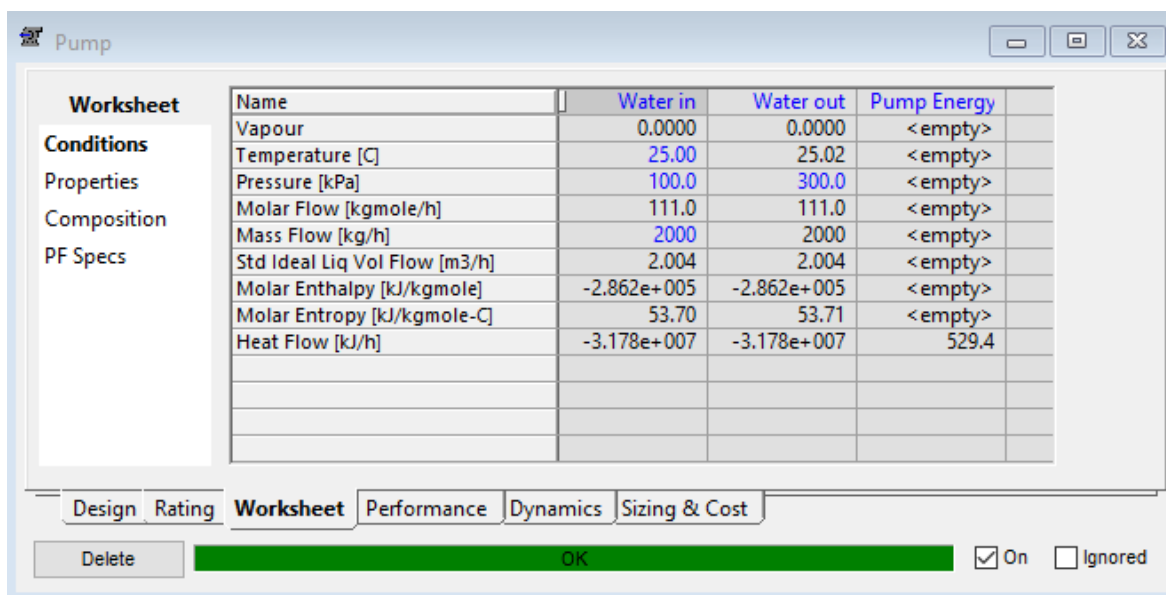


Fig. 4.1: Schematic representation of a shell and tube heat exchanger

Procedure:

- Get started with the UNISIM Design Software
- Add the components involved in the process. Here air and water were added.
- Select the suitable fluid package to analyze the properties of the system. Peng-Robinson package was selected.
- Enter the simulation environment.
- Select the pump from the palette and the inlets and outlets streams are defined.
- The feed conditions are entered and simulated the pump.

7. Select the heater from the palette and the outlet stream of the pump is connected as heater inlet and outlet stream was defined.
8. The heater outlet stream temperature is entered as per the data given in the question.
9. The heat exchanger is added from the palette and the inlets and outlets streams for shell side are defined.
10. Enter the initial feed conditions for shell side based on the data given (minimum 3 conditions).
11. Compositions of the inlet feed was also entered as given in the problem statement.
12. In the parameters tab enter the shell side pressure drop, and tube side pressure drop was entered. (If the data is not given suitable value should be taken (minimum pressure should be given)).
13. Select the worksheet tab and predict the tube side outlet temperature to simulate the heat exchanger and note down the shell side inlet temperature and overall heat transfer coefficient.
14. Report all the condition table for the case.
15. Repeat the step 9, by predicting the shell side inlet temperature and simulate the heat exchanger.
16. Report all the condition table for the case.



Worksheet	Name	Water in	Water out	Pump Energy
Conditions	Vapour	0.0000	0.0000	<empty>
Properties	Temperature [C]	25.00	25.02	<empty>
Composition	Pressure [kPa]	100.0	300.0	<empty>
PF Specs	Molar Flow [kgmole/h]	111.0	111.0	<empty>
	Mass Flow [kg/h]	2000	2000	<empty>
	Std Ideal Liq Vol Flow [m3/h]	2.004	2.004	<empty>
	Molar Enthalpy [kJ/kgmole]	-2.862e+005	-2.862e+005	<empty>
	Molar Entropy [kJ/kgmole-C]	53.70	53.71	<empty>
	Heat Flow [kJ/h]	-3.178e+007	-3.178e+007	529.4

Design Rating **Worksheet** Performance Dynamics Sizing & Cost

Delete OK ☒ On ☐ Ignored

Fig. 4.2: Condition table for Pump

Table – 4.1: Condition table for pump

Name of the Variables	Water in	Water Out	Pump Energy
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: Condition table for heater

Name of the Variables	Water Out	Hot Water in	Heater Energy
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)			

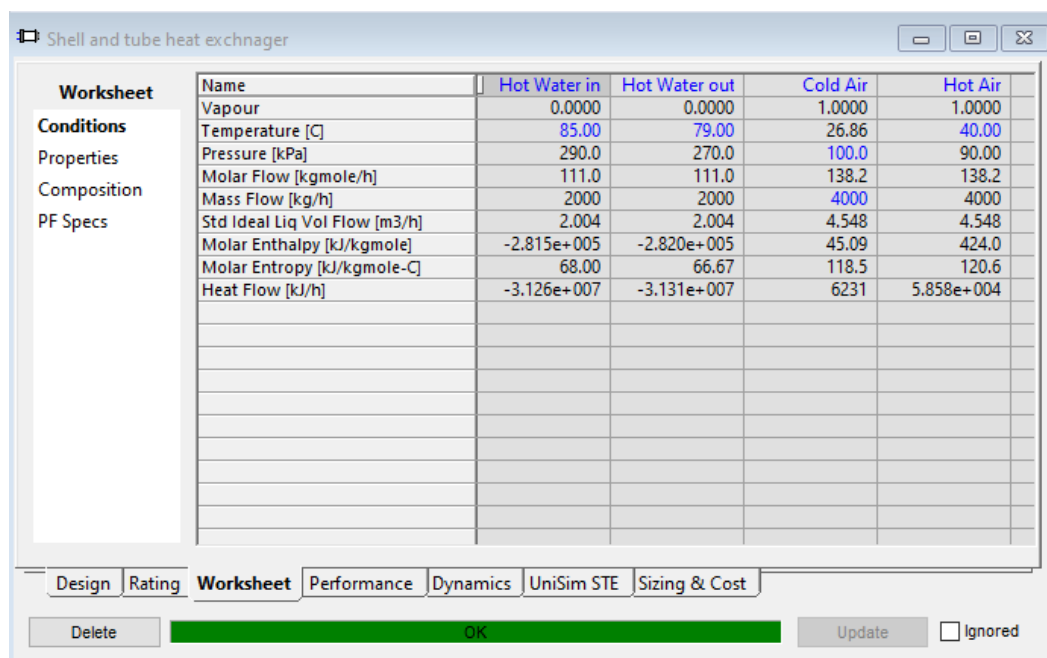


Fig. 4.3: Condition table for heat exchanger

Table – 4.3: Condition table for heat exchanger for fixed tube outlet temperature

Name of the Variables	Hot Water in	Hot Water Out	Cold Air in	Hot Air 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: Condition table for heat exchanger for fixed shell inlet temperature

Name of the Variables	Hot Water in	Hot Water Out	Cold Air in	Hot Air 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)				

Inference:

Experiment No 5

Simulation of two stage compression system

Problem Statement: Simulate the two-stage compression system using a Unisim simulation tool. The humidified air is compressed in compressor 1. The air enters the compressor at 25 °C, and 1 atm pressure. The air flow rate is around 100 kmol/h. Humidity of the air is 50%. The compression ratio for both compressors is 3. The outlet temperature of the air in the heat exchangers 1 and 2 are 30 °C. The pressure drop value in both heat exchangers are 0.1 atm. The cooling water flows at rate of 2000 kmol/h at 25 °C and 1 atm pressure. Use PRSV fluid package.

Tabulate all the simulated conditions for compressor 1, compressor 2, heat exchanger 1 and heat exchanger 2.

Process flow diagram:

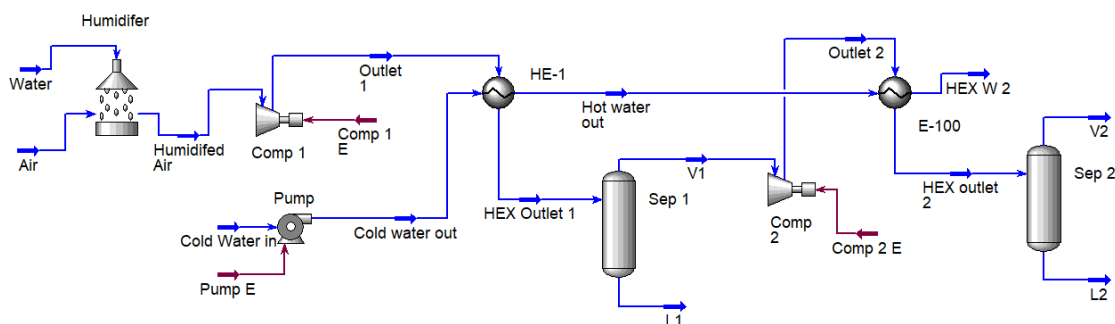


Fig. 5.1: Schematic representation of a two-stage compressor system.

Procedure:

1. Get started with the UNISIM Design Software
2. Add the components involved in the process. Here air and water were added.
3. Select the suitable fluid package to analyze the properties of the system. PRSV package was selected.
4. Enter the simulation environment.
5. From the flowsheet tab, select add operations and select the saturate operation in the list and the inlets and outlets streams are defined.
6. Connect the humidifier outlet to compressor 1 and give the conditions.
7. Select the pump from the palette and the inlets and outlets streams are defined.

8. The feed conditions are entered and simulated the pump.
9. Add heat exchanger and allow the compressor 1 outlet to shell side and outlet of the pump to the tube side.
10. Add a separator and simulate the process.
11. The vapour outlet of separator 1 is connected to compressor 2 and simulated with the data provided.
12. The heat exchanger is added from the palette and the inlets and outlets streams for shell side and tube side are defined.
13. Add a separator and simulate the process.
14. Compositions in both separators are tabulated.

Table – 5.1: Condition table for compressor 1

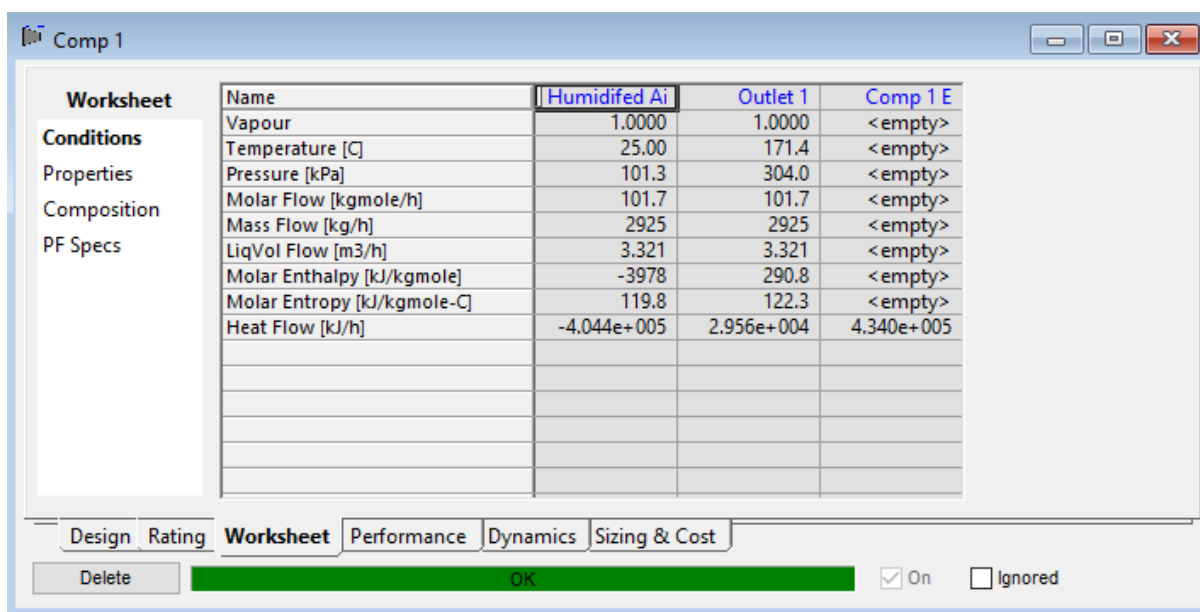
Name of the Variables	Humidified Air	Outlet 1	Comp 1 E
Vapour			
Temperature (°C)			
Pressure (kPa)			
Molar flow rate (kmol/h)			
Mass flow rate (kg/h)			
Std. ideal liquid Vol flow (m ³ /h)			
Molar Enthalpy (KJ/kgmol. °C)			
Molar Entropy (KJ/kgmol. °C)			
Heat Flow (KJ/h)			

Table – 5.2: Condition table for Heat exchanger 1

Name of the Variables	Cold water out	Hot water out	Outlet 1	HEX Outlet 1
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)				

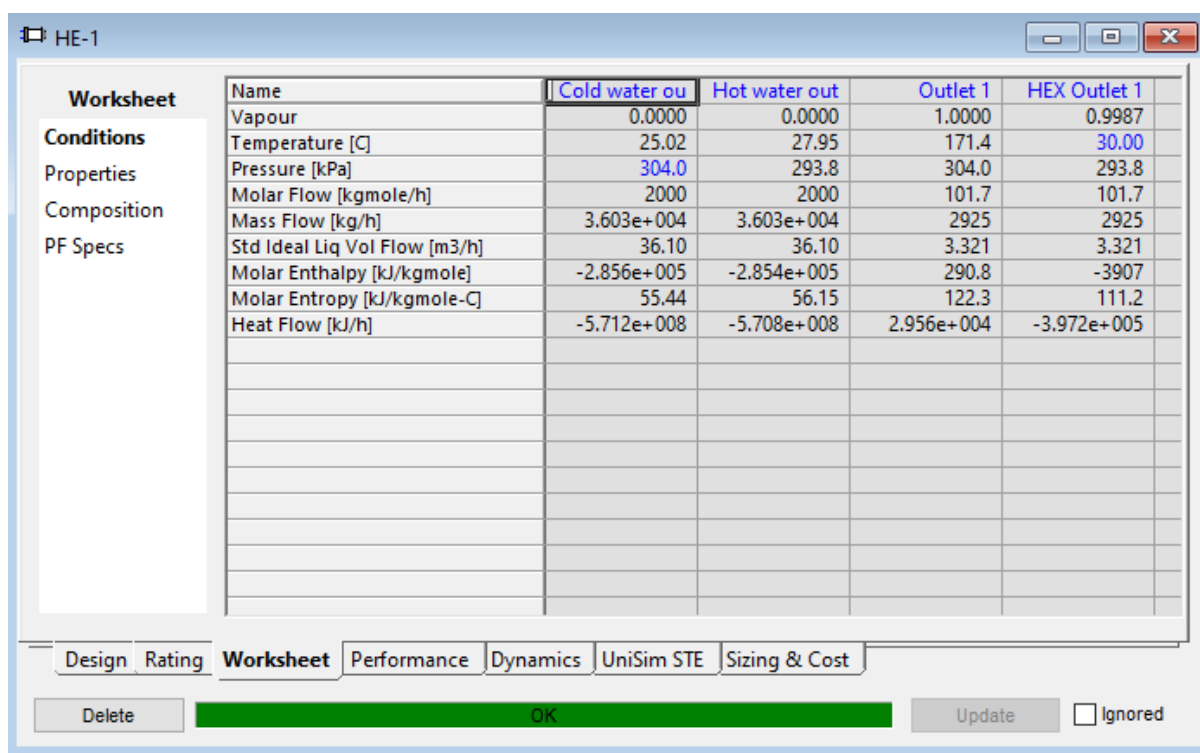
Table – 5.3: Composition table at Separator 1

Components	HEX Outlet 1	L1	V1
Water			
Air			



Name	Humidified Ai	Outlet 1	Comp 1 E
Vapour	1.0000	1.0000	<empty>
Temperature [C]	25.00	171.4	<empty>
Pressure [kPa]	101.3	304.0	<empty>
Molar Flow [kgmole/h]	101.7	101.7	<empty>
Mass Flow [kg/h]	2925	2925	<empty>
LiqVol Flow [m3/h]	3.321	3.321	<empty>
Molar Enthalpy [kJ/kgmole]	-3978	290.8	<empty>
Molar Entropy [kJ/kgmole-C]	119.8	122.3	<empty>
Heat Flow [kJ/h]	-4.044e+005	2.956e+004	4.340e+005

Fig. 5.2: Condition table for compressor 1.



Name	Cold water ou	Hot water out	Outlet 1	HEX Outlet 1
Vapour	0.0000	0.0000	1.0000	0.9987
Temperature [C]	25.02	27.95	171.4	30.00
Pressure [kPa]	304.0	293.8	304.0	293.8
Molar Flow [kgmole/h]	2000	2000	101.7	101.7
Mass Flow [kg/h]	3.603e+004	3.603e+004	2925	2925
Std Ideal Liq Vol Flow [m3/h]	36.10	36.10	3.321	3.321
Molar Enthalpy [kJ/kgmole]	-2.856e+005	-2.854e+005	290.8	-3907
Molar Entropy [kJ/kgmole-C]	55.44	56.15	122.3	111.2
Heat Flow [kJ/h]	-5.712e+008	-5.708e+008	2.956e+004	-3.972e+005

Fig. 5.3: Condition table for Heat exchanger 1.

Table – 5.4: Condition table for compressor 2

Name of the Variables	V1	Outlet 2	Comp 2 E
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 – 5.5: Condition table for Heat exchanger 2

Name of the Variables	Hot water out	HEX W 2	Outlet 2	HEX outlet 2
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 – 5.6: Composition table at Separator 2

Components	HEX Outlet 2	L2	V2
Water			
Air			

Inference:

Experiment No 6

Simulation of refrigeration gas plant

Problem Statement: 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

- Quality of the evaporator inlet
- Rate of heat transfer to the evaporator
- Mass flow of cold water in the condenser and evaporator.
- 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:

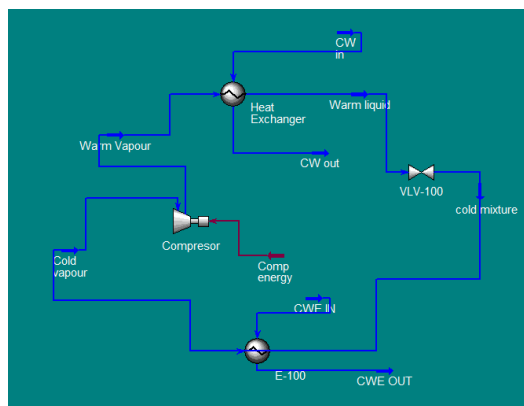


Fig. 6.1: Process flow diagram for refrigeration cycle

Procedure:

- Open new simulation, select a suitable fluid package (Peng Robinson and SRK models) add the components required.
- Enter the simulation environment and add the compressor operation, define the streams and conditions provided.
- Enter all the details given in the problem.
- Select the condenser from the object palette and connect warm vapor as tube side inlet and cold water as shell side inlet.
- 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

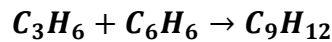
Material Streams	Components	Composition in mole fractions
Cold Mixture	R-134a	
	Water	
Cold Vapour	R-134a	
	Water	
Water in	R-134a	
	Water	
Water out	R-134a	
	Water	

Inference:

Experiment No 7

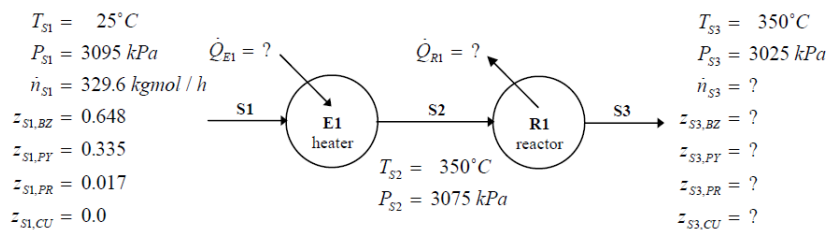
Simulation of conversion reactor

Problem Statement: 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:

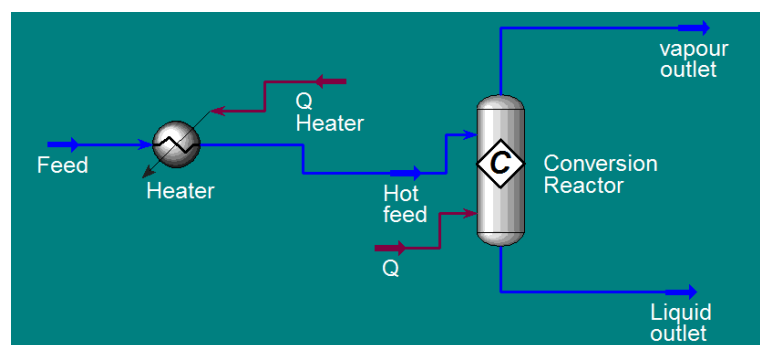


Fig 7.1: Conceptual model of the heater and reactor system

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.

3. Enter the simulation environment and select the Heater unit from the object palette.
4. Name the material streams and Energy stream required.
5. 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 –7.1: 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 –7.2: 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)			

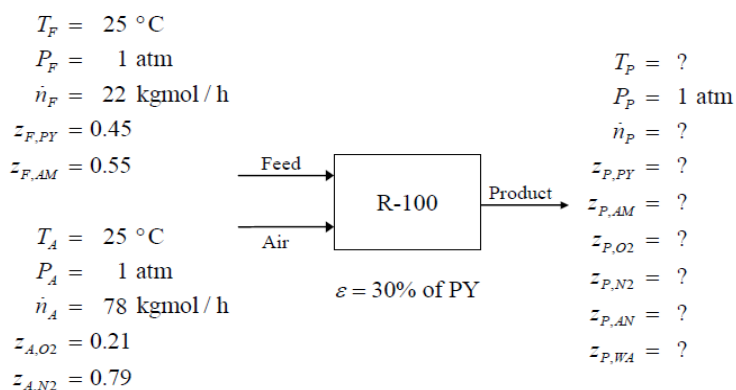
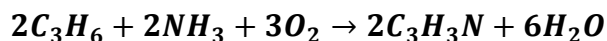
Table – 7.3: Composition table for Conversion Reactor

Components	Hot Feed	Liquid Outlet	Vapour Outlet
Propene			
Benzene			
Cumene			
Propane			

Inference:

Problem Statement: Let 45 mole% propylene and 55 mole % ammonia streams 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:

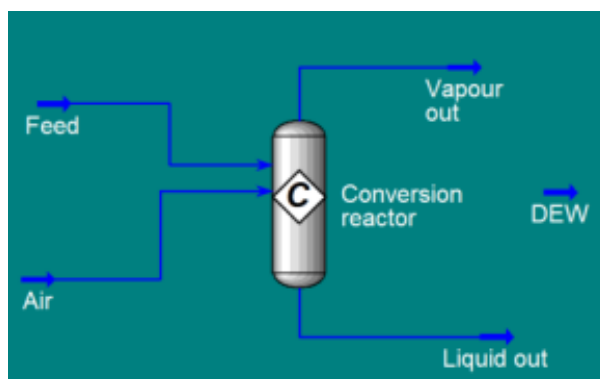


Fig 7.4: Conceptual model of the reactor

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 –7.5: 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 – 7.6: Composition table for Conversion Reactor

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

Result Table	
Product Outlet temperature	
Dew point of product stream	

Inference:

Experiment No 8

Simulation of equilibrium reactor

Problem Statement: Hydrogen is produced using water gas shift reaction at temperature around 250 °C and 10 atm pressure. Here carbon monoxide will react with water to give carbon dioxide and hydrogen. Water is stored in a tank at 25 °C and 1 atm pressure. This water is pumped from a storage tank into the heater to by increasing the pressure to 2 atm and heated to 100°C. The water flow rate 100 kmol/h. Carbon Monoxide enter the reactor at 2 atm pressure at rate of 100kmol/h. Simulate the given reaction using equilibrium reactor in Unisim simulation software.

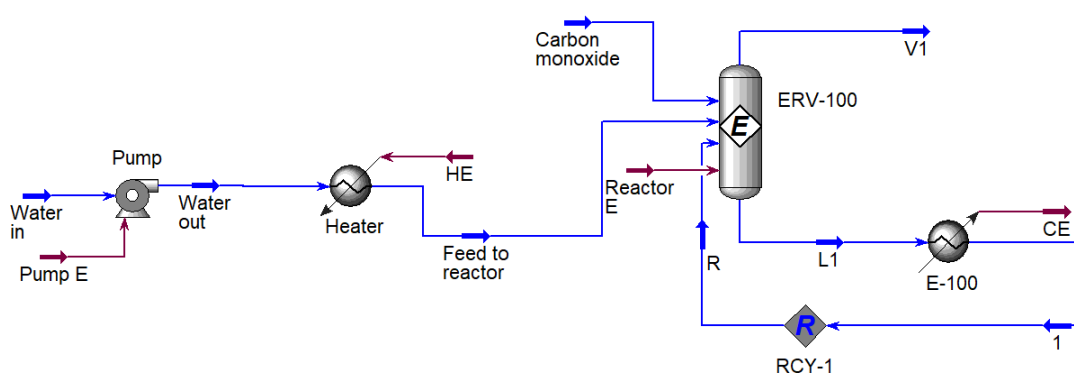


Fig 8.1: Conceptual model of the equilibrium reactor

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 equilibrium reaction. Enter the stoichiometric coefficients.
3. Attach the reaction set to the selected fluid package.
4. Enter the simulation environment and select the pump first to pump water from storage tank.
5. Name the material streams and energy stream required as shown in the process flow diagram for pump.
6. Enter the feed stream conditions, and other conditions specified in the problem.
7. Add a heater operation and connect the pump outlet to the heater as shown in PFD.
8. Select equilibrium reactor from the object palette, name the carbon monoxide stream and enter the inlet conditions. Add the heater outlet stream as other inlet into the reactor.

9. Check the composition of the vapour and liquid stream of the reactor. Recycle the excess reactant water back to the reactor by cooling to 100 °C.
10. Tabulate the results obtained.

ERV-100 - Global Rxn Set

Worksheet	Name	Feed to react	Carbon mono	R	L1	V1	Reactor E
Conditions	Vapour	0.0000	1.0000	0.0875	0.0000	1.0000	< empty >
	Temperature [C]	100.0	-163.3	100.0	250.0	250.0	< empty >
Properties	Pressure [kPa]	1003	1013	1003	1003	1003	< empty >
	Molar Flow [kgmole/h]	100.0	100.0	0.0000	0.0000	200.0	< empty >
Composition	Mass Flow [kg/h]	1802	2801	0.0000	0.0000	4603	< empty >
	Std Ideal Liq Vol Flow [m3/h]	1.805	3.504	0.0000	0.0000	7.947	< empty >
PF Specs	Molar Enthalpy [kJ/kgmole]	-2.803e+005	-1.166e+005	-2.822e+005	-2.679e+005	-1.872e+005	< empty >
	Molar Entropy [kJ/kgmole-C]	71.27	107.5	79.11	108.4	158.2	< empty >
	Heat Flow [kJ/h]	-2.803e+007	-1.166e+007	-0.0000	-0.0000	-3.743e+007	2.261e+006

Design Reactions Rating **Worksheet** Dynamics

Delete OK Ignored

Fig 8.2: Condition table for equilibrium reactor

The screenshot shows the "ERV-100 - Global Rxn Set" dialog box. The "Worksheet" tab is active, displaying a table with columns: Feed to reactor, Carbon monoxide, R, L1, V1, and an unlabeled column. The rows are categorized by Conditions, Properties, Composition, and PF Specs.

	Feed to reactor	Carbon monoxide	R	L1	V1	
H ₂ O	1.000000	0.000000	0.920971	0.920971	0.046539	
Hydrogen	0.000000	0.000000	0.015442	0.015442	0.453461	
CO ₂	0.000000	0.000000	0.061946	0.061946	0.453461	
CO	0.000000	1.000000	0.001641	0.001641	0.046539	

At the bottom, there are tabs for Design, Reactions, Rating, **Worksheet**, and Dynamics. A green bar at the very bottom contains a Delete button, OK, and Ignored checkbox.

Fig 8.3: Composition table for equilibrium reactor

Table –8.1: Condition table for equilibrium reactor

Name of the Variables	Feed to reactor	Carbon monoxide	R	L1	V1	Reactor E
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: Composition table for equilibrium reactor

Components	Feed to reactor	Carbon monoxide	R	L1	V1
Hydrogen					
Carbon monoxide					
Carbon dioxide					
water					

Inference:

Experiment No 9

Simulation of CSTR

Problem Statement: The hydrogenation of aniline produces cyclohexylamine in a CSTR. The reaction is represented as $\text{C}_6\text{H}_5\text{NH}_2 + 3\text{H}_2 \rightarrow \text{C}_6\text{H}_{11}\text{NH}_2$. The reactor operates at 40 bar and 100 °C. The volume of the reactor is 34 m³. The reactant pure aniline enters at 43 °C and 41 bar at a rate of 45 kmol/h and pure hydrogen enters at 230 °C and 41 bar at a rate of 140 kmol/h into the reactor. Develop a process flow diagram for the process and simulate the same using suitable fluid package. Estimate the following.

- The conditional table for the CSTR
- The conversion percentage, and extent of reaction.
- The liquid and vapour product stream compositions for initial volume and optimized volume.

Data: Pre-exponential Factor $A = 5 \times 10^5 \text{ m}^3/\text{kmol s}$; Activation Energy $E = 4.65 \times 10^4 \text{ kJ/kmol}$.

Process flow diagram:

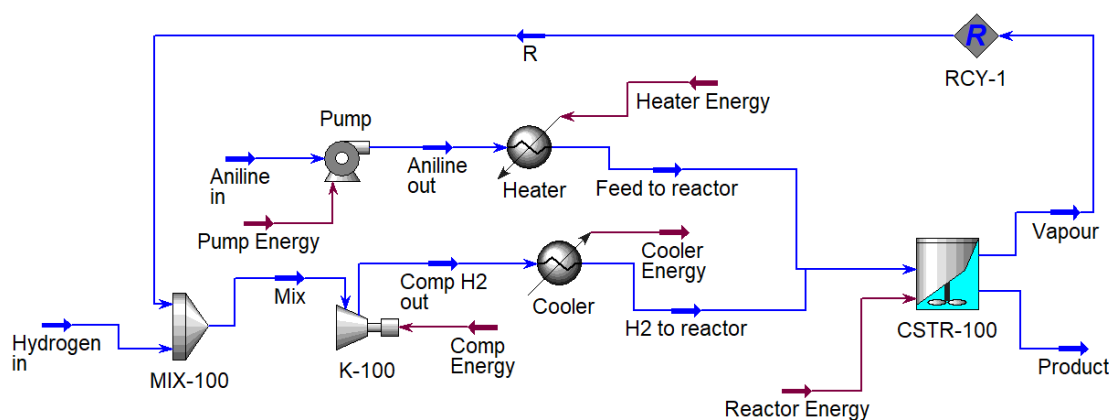


Fig 9.1: Conceptual model of the reactor

Procedure:

- Open new simulation file, select a suitable fluid package and the components required.
- Define the reaction given in the reaction tab as kinetic reaction. Enter the Activation energy and pre-exponential factor as reaction parameters.
- Attach the reaction set to the selected fluid package.
- Enter the simulation environment and select the pump first to pump aniline from storage tank.

5. Name the material streams and energy stream required as shown in the process flow diagram for pump.
6. Enter the feed stream conditions, and other conditions specified in the problem.
7. Add a heater operation and connect the pump outlet to the heater as shown in PFD.
8. Select mixer and compressor operation from the object palette, name the streams and enter the inlet conditions for mixer and connect the mixer outlet to the compressor.
9. Select CSTR from the object palette, name the streams and attach the inlet streams to the reactor.
10. Enter the reactor volume in rating tab and add the reaction set to the reactor.
11. Check the composition of the vapour and liquid stream of the reactor. Recycle the excess reactant hydrogen back to the mixer unit before compressor.
12. Tabulate the results obtained.

CSTR-100 - Global Rxn Set

Worksheet

Conditions

Properties

Composition

PF Specs

Name	Feed to reactor	H2 to reactor	Product	Vapour	Reactor Energy
Vapour	0.0000	1.0000	0.0000	1.0000	<empty>
Temperature [C]	45.00	500.0	100.0	100.0	<empty>
Pressure [kPa]	4100	4100	4000	4000	<empty>
Molar Flow [kgmole/h]	45.00	646.9	45.74	511.1	<empty>
Mass Flow [kg/h]	4191	1827	4460	1558	<empty>
Std Ideal Liq Vol Flow [m3/h]	4.091	19.12	5.074	15.20	<empty>
Molar Enthalpy [kJ/kgmole]	3.960e+004	1.427e+004	-5.935e+004	1862	<empty>
Molar Entropy [kJ/kgmole-C]	-86.30	157.4	-184.2	134.6	<empty>
Heat Flow [kJ/h]	1.782e+006	9.233e+006	-2.715e+006	9.515e+005	-1.278e+007

Design

Reactions

Rating

Worksheet

Dynamics

Cost

Delete

OK

Ignored

Fig 9.2: Conditional table for CSTR

Table –9.1: Condition table for CSTR

Name of the Variables	Feed to reactor	H ₂ to reactor	Product	Vapour	Reactor Energy
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)					

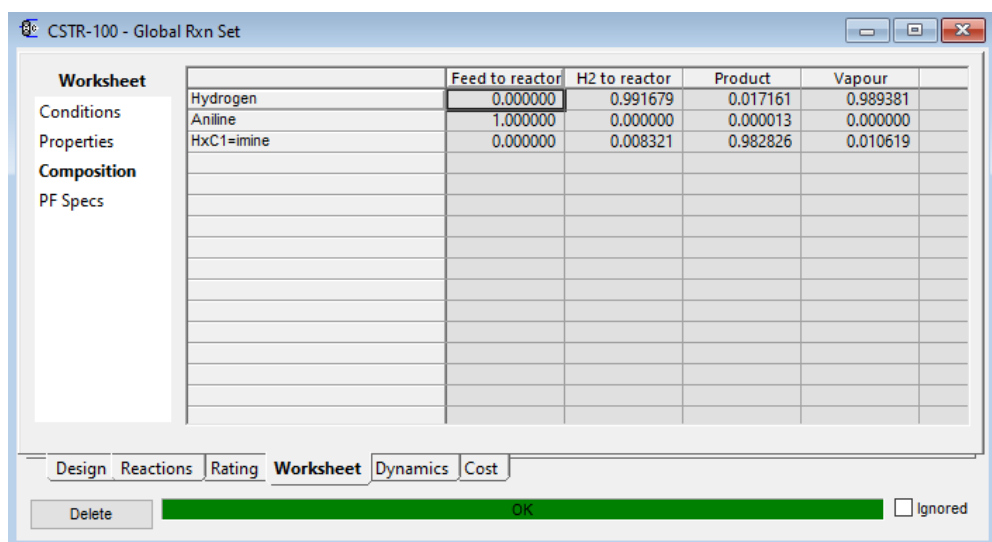


Fig 9.3: Composition table for CSTR

Table – 9.2: Composition table for CSTR

Components	Feed to reactor	H ₂ to reactor	Product	Vapour
Aniline				
Hydrogen				
Cyclohexylamine				

Inference:

Experiment No 10

Simulation of Plug Flow Reactor

Problem Statement: The hydrogenation of aniline produces cyclohexylamine in a PFR. The reaction is represented as $\text{C}_6\text{H}_5\text{NH}_2 + 3\text{H}_2 \rightarrow \text{C}_6\text{H}_{11}\text{NH}_2$. The reactor operates at 40 bar and 100 °C. The volume of the reactor is 34 m³. The reactant pure aniline enters at 43 °C and 41 bar at a rate of 45 kmol/h and pure hydrogen enters at 230 °C and 41 bar at a rate of 140 kmol/h into the reactor. Develop a process flow diagram for the process and simulate the same using suitable fluid package. Estimate the following.

- The conditional table for the PFR
- The conversion percentage, and extent of reaction.
- The liquid and vapour product stream compositions for initial volume and optimized volume.

Data: Pre-exponential Factor $A = 5 \times 10^5 \text{ m}^3/\text{kmol s}$; Activation Energy $E = 4.65 \times 10^4 \text{ kJ/kmol}$.

Process flow diagram:

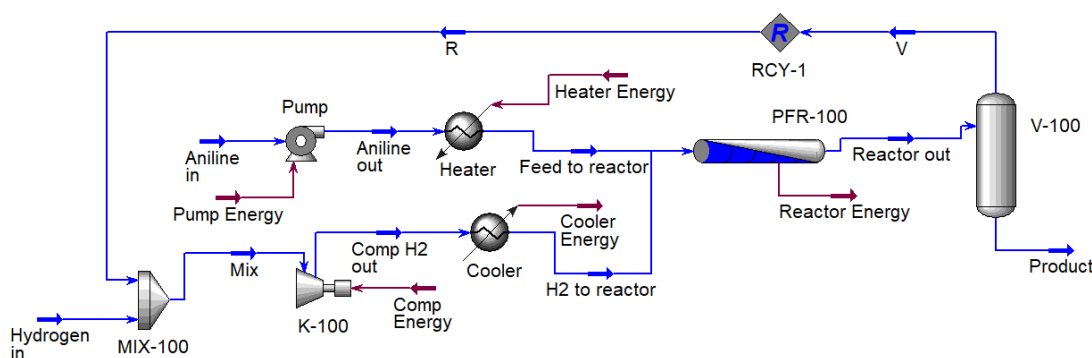


Fig 10.1: Conceptual model of the PFR

Procedure:

- Open new simulation file, select a suitable fluid package and the components required.
- Define the reaction given in the reaction tab as kinetic reaction. Enter the Activation energy and pre-exponential factor as reaction parameters.
- Attach the reaction set to the selected fluid package.
- Enter the simulation environment and select the pump first to pump aniline from storage tank.

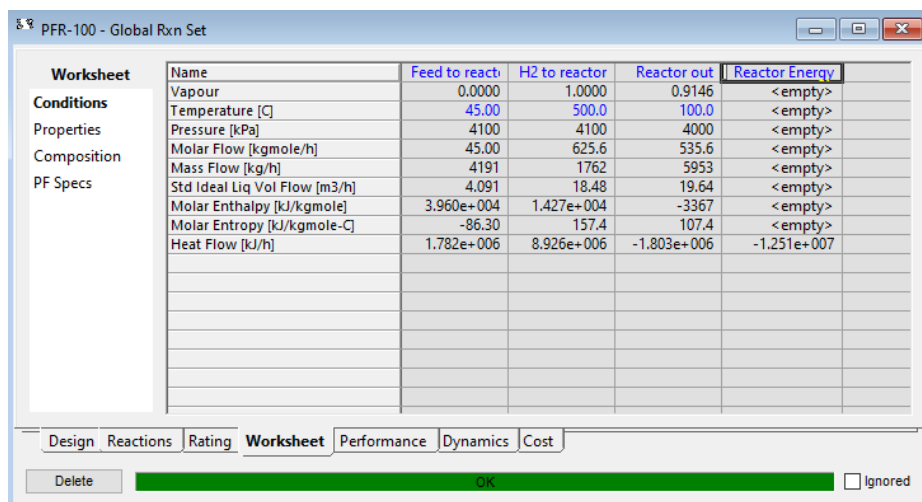
5. Name the material streams and energy stream required as shown in the process flow diagram for pump.
6. Enter the feed stream conditions, and other conditions specified in the problem.
7. Add a heater operation and connect the pump outlet to the heater as shown in PFD.
8. Select mixer and compressor operation from the object palette, name the streams and enter the inlet conditions for mixer and connect the mixer outlet to the compressor.
9. Select PFR from the object palette, name the streams and attach the inlet streams to the reactor.
10. Enter the reactor volume in rating tab and add the reaction set to the reactor.
11. Check the composition of the vapour and liquid stream of the reactor. Recycle the excess reactant hydrogen back to the mixer unit before compressor.
12. Tabulate the results obtained.

Table –10.1: Condition table for PFR

Name of the Variables	Feed to reactor	H ₂ to reactor	Reactor Out	Reactor Energy
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)				

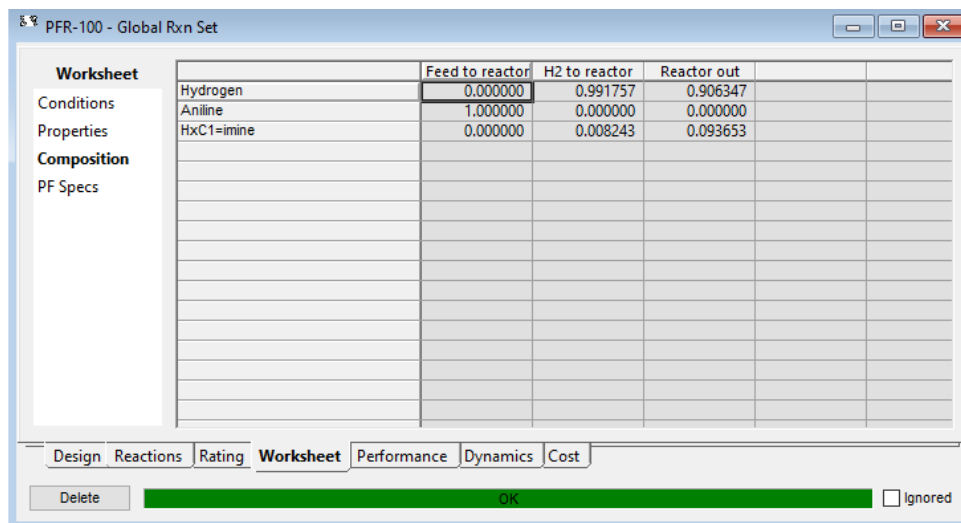
Table – 10.2: Composition table for CSTR

Components	Feed to reactor	H ₂ to reactor	Reactor Out
Aniline			
Hydrogen			
Cyclohexylamine			



Worksheet	Name	Feed to reactor	H2 to reactor	Reactor out	Reactor Energy
Conditions	Vapour	0.0000	1.0000	0.9146	<empty>
	Temperature [C]	45.00	500.0	100.0	<empty>
Properties	Pressure [kPa]	4100	4100	4000	<empty>
	Molar Flow [kgmole/h]	45.00	625.6	535.6	<empty>
Composition	Mass Flow [kg/h]	4191	1762	5953	<empty>
	Std Ideal Liq Vol Flow [m3/h]	4.091	18.48	19.64	<empty>
PF Specs	Molar Enthalpy [kJ/kgmole]	3.960e+004	1.427e+004	-3367	<empty>
	Molar Entropy [kJ/kgmole-C]	-86.30	157.4	107.4	<empty>
	Heat Flow [kJ/h]	1.782e+006	8.926e+006	-1.803e+006	-1.251e+007

Fig 10.2: Conditional table for PFR



Worksheet		Feed to reactor	H2 to reactor	Reactor out
Conditions	Hydrogen	0.000000	0.991757	0.906347
	Aniline	1.000000	0.000000	0.000000
	HxC1=imine	0.000000	0.008243	0.093653
Composition				

Fig 10.3: Composition table for PFR

Inference: