EXERCISE - 1

Thermodynamic Properties

(a) Estimate all the physical properties of a component, for which no data is available in the data base of the simulators.

Example: (i) CH_3CHCH_2OH
CH_3

(ii) CH_3-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-OH

H3C
(iii) H3C – C - O – CH3 (MTBE)

(b) Plot the molar volume of any pure component as a function of temp at a given pressure.

(c) For the following binary systems generate the VLE data and plot T-x-y and P-x-y plots. Try to use different thermodynamic property methods and analyze the results.

i. Methyl ethyl ketone (1) and toluene (2)
ii. Chloroform (1) and 1,4-dioxane (2)
iii. Chloroform (1) and Tetrahydrofuran (2)
iv. Ethanol (1) and Toluene (2)

(d) Learn to plot the ternary diagram (LLE) and residue curves for the following systems and comment whether the chosen solvent is good for separation:

i) Ethanol, Water and Cyclohexane
ii) Acetone, Water and 3-Methylhexane

(e) For a binary system involving one user defined component and another component from the data bank, generate the VLE data and plot T-x-y and P-x-y plots.

(f) For any binary / multi-component system, plot the bubble point and dew point temperatures, as a function of pressure.

(g) For any binary / multi-component system with known composition at a given temperature and pressure, generate a report with the required physical properties.

(h) For any binary / multi-component system, calculate the bubble P, dew P, bubble T and dew T giving the respective inputs in each case.

EXERCISE – 2

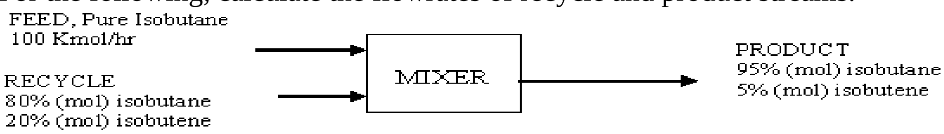
Mixers & Splitters:

a) Simulate **MIXER**, with input streams (two or more) and one output stream.

b) Simulate **FLOW SPLITTER**, with one input stream and (two or more) output streams.

c) Simulate the unit, **COMPONENT SEPARATOR**, with one input stream and two or more output streams.

d) For the following, calculate the flowrates of recycle and product streams.



e) 1000 lb/hr of toluene stream (S1) at 100 ^{0}F is mixed with ethylene stream (S2). The flow rate of the ethylene stream which is at 50 ^{0}F is adjusted to achieve the desired temperature of 85 ^{0}F at the mixer effluent. Both the input streams may be assumed to be at a pressure of 1 atm. Simulate the unit and find the flow rate of the stream S2.

Decanter:

A 100 kmol/hr feed stream that is 35 mol % ethanol, 6 mol % water, and 59 mol % cyclohexane is fed to a decanter at 25 ^{0}C ad 1 atm. Determine the compositions of the two outlet streams from the decanter and their flowrates.

Pumps

1. Water at 60 ^{0}F is to be pumped from a reservoir to the top of a mountain through a 6-in steel (schedule 120) pipe at a rate of 200 gal/min. The pipe discharges into the atmosphere at a level of 3000 ft above the level in the reservoir. The pipe line is 4500 ft long and contains two gate valves, four standard tees and four elbows. Suggest the rating of the pump required to meet the above purpose.
2. 5 ft^3/s of water at 10 bar and 25 ^{0}C is to be routed through 2 different pipes (pipe-1: dia= 4 in; equivalent length = 20 ft and pipe -2: dia = 2 in; equivalent length = 22 ft). Simulate to find the fraction of the total water flow that passes through pipe-2.
3. 25,000 lb/hr of toluene is pumped from 75 ^{0}F and 30 psi to 570 psi. Simulate to compute the capacity, the pump head, the exit temperature and horse power for (a) a pump efficiency of 100% and (b) a pump efficiency of 75%.

Heat Exchangers

a) Select a heater/shell and tube heat exchanger model and perform rating/simulation calculations taking a suitable example.

b) Process fluid consisting of Methanol 36.8% and Water 63.2 mole% has to be heated from 25 ^{0}C to 70^{0}C at the rate of 1000 mol/hr. Design a shell and tube heat exchanger.

c) Freon-12 (Dichlorodifluoromethane), at a flow rate of 10560 kg/hr, needs to be heated from 240 K to 300 K at a pressure of 7 atm. Ethylene glycol is available at 350 K and 2 atm. A typical shell and tube heat exchanger will be used. The plant manager recommends that the exit temperature of ethylene glycol can be at 320K. It is also recommended that the pressure drop shall not exceed 10 psig (0.67 atm) for either the shell or tube side. Perform a detailed design of a shell and tube heat exchanger.

d) Water is to be heated from 25 ^{0}C to 80 ^{0}C at 1 atm. Two streams of steam (H_1 and H_2), one at 120 ^{0}C and the other at 110 ^{0}C are available, both at a pressure of 5 bar. The flow rates of all the three streams are same and equal to 1000 kg/h. The cold stream can first pick up heat from H_1 followed by H_2, or from H_2 followed by H_1. Simulate to find the exit temperature of water from the first exchanger that minimizes the total area for both the sequences: H1 followed by H2 and H2 followed by H1. Which of these two sequences are better and why?

EXERCISE – 3: Reactors

1. Calculate the standard heat of reaction for $CO + 2H_2 \rightarrow CH_3OH$ and compare the result obtained from standard heats of formation.
2. Calculate the adiabatic reaction temperature for the reaction $CO + 2H_2 \rightarrow CH_3OH$ under the following conditions. The feed consisting of CO and H_2 in the stoichiometric ratio enters the reactor at 25 ^{0}C and 1 atm. A conversion of 80% with respect to CO may be assumed. Compare the result with conventional calculation. What will be this temperature if CO and H_2 in the mole ratio of 1:10 enter the reactor.
3. The gas phase reversible reaction $C_3H_8 \leftrightarrow C_2H_4 + CH_4$ is allowed to reach equilibrium starting with pure C_3H_8 at a pressure of 1 atm. Simulate to find the temperature at which the reactor must operate in order to obtain a conversion of 80% at equilibrium. Use Equilibrium / Gibbs reactor models and compare the result.
4. Consider the elementary reversible liquid phase esterification of acetic acid shown below: Acetic acid + ethanol $\Leftrightarrow$ ethyl acetate + water. $K_f = 8 \times 10^{-6}$ m^3/kmol/s; $K_r = 2.7 \times 10^{-6}$ m^3/kmol/s. Determine the time required using a batch reactor to achieve 30% reaction conversion given an initial charge of 1,045 kg containing 13 mol % acetic acid, 35 mole % ethanol, and 52 mole % water.
5. Feed consisting of Hydrogen = 2049.0, Methane = 3020.8, Benzene = 39.846, Toluene = 362 lbmol/hr enters into a Toluene Hydrodealkylation Reactor at 1200 F and 494 psi. The reaction $H_2 + C_7H_8 \rightarrow CH_4 + C_6H_6$ may be assumed to be first order with respect to toluene and 0.5 order with respect to hydrogen. The frequency factor and activation energy for the reaction are: 6.3×10^{10} and 52000 cal/mol respectively. Design an adiabatic plug flow reactor for obtaining a conversion of 25% of toluene.
6. Perform Design calculations with any kinetic reactor (PFR / CSTR). Determine the volume necessary to produce 300 million pounds of ethylene a year from cracking a feed stream of pure ethane. The reaction is irreversible and elementary. It is required to obtain 60% conversion of ethane, operating the reactor isothermally at 1150K and a pressure of 5 atm.

$$C_2H_6\ (g) \rightarrow C_2H_4\ (g) + H_2\ (g)\ (A \rightarrow B + C)$$

DATA: $k = 0.072 s^{-1}$ at 1000K and Activation Energy, E = 82 kcal/gmol

7. For the data given above, compare the conversions obtained in an isothermal reactor with that obtained in an adiabatic reactor (PFR/CSTR). Use equal volumes for both isothermal operation and adiabatic operation.
8. For the kinetic data given above and for a pure C_2H_6 flowrate of 1 kmol/s, simulate and compare the exit conversions obtained in each of the following:
   a) A single CSTR of 3 m^3 volume (b) A single PFR of equal volume (c) Two CSTRs of volume 1.5 m^3 each connected in series (d) A CSTR (1.5 m^3) followed by a PFR (1.5 m^3). (e) A PFR (1.5 m^3) followed by a CSTR (1.5 m^3) (f) A battery of 6 CSTRs (each of 0.5 m^3).

   Simulate all the above i.e., (a) to (f) in the same problem.

EXERCISE – 4: FLASH COLUMNS

1. An equimolar binary mixture of toluene and benzene at 1 bar and 25°C is to be fed into a flash column. Examine the following flash conditions:
   a) (**P-V Flash**): At 1 bar and a vapor fraction of 0.5, find the temperature and the heat duty.
   b) (**T-P Flash**): At the temperature determined from (a) and a pressure of 1 bar, verify the flash model results in a vapor fraction of 0.5 at equilibrium.
   c) (**T-V Flash**): At the temperature of (a), and a vapor fraction of 0.5, verify that the flash model results in an equilibrium pressure of 1 bar.
   d) (**P-Q Flash**): At 1 bar and with the heat duty determined from (a), verify that the temperature and vapor fraction are consistent with previous conditions.
   e) (**T-Q Flash**): At the temperature and heat duty determined from (a), verify that the pressure and vapor fraction are consistent with previous conditions.
2. A binary mixture consisting of 50 mol% N-Pentane and 50 mol% N-Hexane at 130 ^{0}F and 73.5 psi is fed into a flash column. The flash column operates at 120 ^{0}F and 13.23 psi pressure. Simulate the unit and report the fraction of vapor along with the compositions of the liquid and vapor streams. Observe the heat duty in the column. Try to connect a Heat stream to the column and observe its value.
3. (a) Consider the flash separation process shown in the following figure. Solve all the three cases using the RK-Soave option set for thermo-physical properties. Compare and discuss the flow rates and compositions for the overhead stream produced by each of the three cases. (b) Modify case 3 to determine the flash temperature necessary to obtain 850 lb/hr of overhead vapor.
4. The figure shown below represent a process close to distillation operation. Simulate the process as per the details given and determine the flowrates of all the streams in the process.

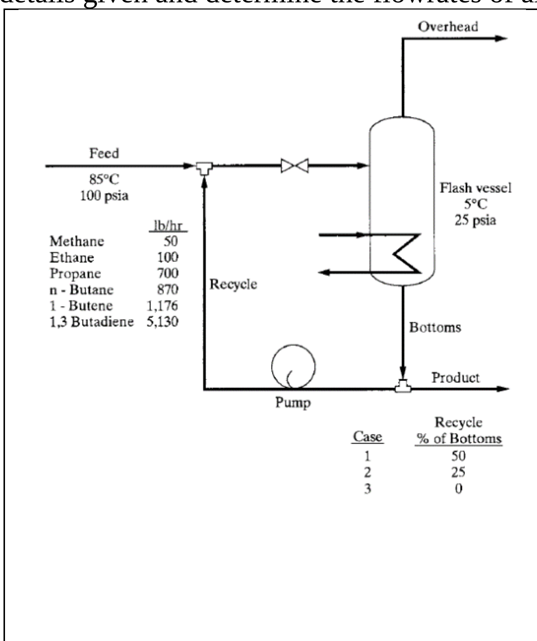


Fig. for Problem (3)

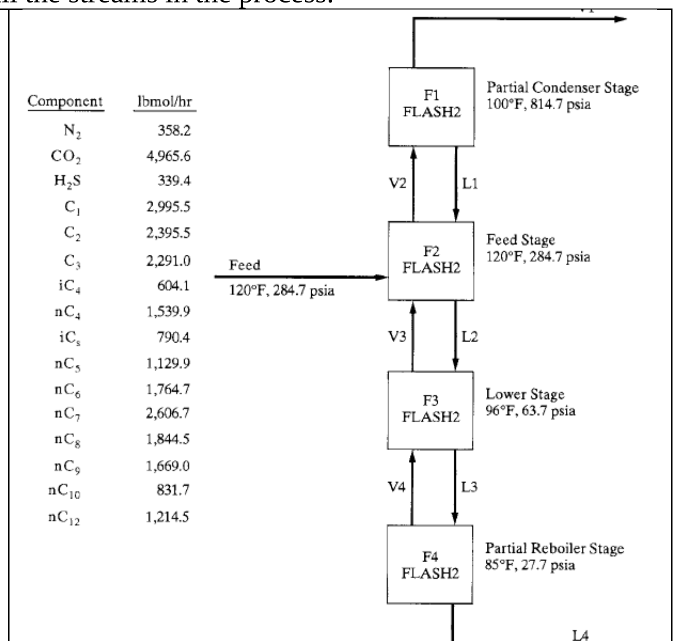


Fig. for Problem (4)

5. A liquid mixture consisting of Benzene, Toluene and O-Xylene enters a flash column operating at 1 bar. The component flowrates of Benzene, Toluene and O-xylene are: 30, 50 and 40 kmol/hr respectively. It is desired to obtain a vapor fraction of 0.8 in the flash column. Simulate the column and report the tempearture at which the flash column must operate.
6. Assume the feed into a flash tank consisting of 25 moles of pentane, 40 moles of cis-2-butene and 35 moles of n-butane. Simulate the column to (i) find the recovery of n-butane when the pressure is 160 kPa and tempearature is 300 K in the flash column. (ii) If the flash tank operates at 100 kPa, at what temperature can the recovery of cis-2-butene be 60% in the vapor phase.

EXERCISE – 5: Material Balances

HINT: For solving these problems select RSTOIC model. Assume the same temperature and pressure for the feed at which the reactor is operating.

1. Methanol is produced by the reaction of CO with H_2 according to the reaction $CO + 2H_2 \rightarrow CH_3OH$. Only 15 % of the CO entering the reactor is converted to methanol. The Methanol produced is separated and the un-reacted gases are recycled. The fresh feed contains 2 mol of H_2 for every mol of CO. Based on 100 mol/hr of fresh feed, calculate: a) the recycle rate b) the product rate.
2. Feed gas consisting of 75.16 mol% H_2, 24.57 % N_2 and 0.27% Ar is mixed with recycle gas and enters into a reactor where 10% of N_2 is converted to NH_3 as per the reaction: $N_2 + 3H_2 \rightarrow 2NH_3$. NH_3 from the exit of the reactor is completely separated from the un-converted gases. In order to avoid the built-up of inerts, a small fraction (5%) of the unreacted gases are purged and the balance recycled. Based on 100 mol/hr of fresh feed, calculate: (a) Recycle rate and composition (b) Product rate and (c) Purge rate.
3. In an ammonia reactor loop, the feed consisting of NITROGEN 24 lbmol/hr, HYDROGEN 74.3 lbmol/hr, ARGON, 0.6 lbmol/hr and METHANE 1.1 lbmol/hr enters a reactor at 77 ^{0}F and 200 atm. The reactor (Modeled as Equilibrium reactor with zero degree temperature approach) is operating at 200 atm and 500 ^{0}C. The vapor and liquid product streams from the reactor are mixed and cooled to -28 ^{0}F and then admitted into a flash column. The flash column is operating at -28 ^{0}F and 2000 psi. The liquid stream from the flash column is withdrawn as product and the vapor stream is partially purged (a purge fraction of 0.04 may be used) and then compressed to the reactor pressure of 200 atm. Simulate the process and report the conversion obtained in the reactor along with the product and recycle flow rates.
4. In the feed preparation section of a plant ethyl benzene at 77 ^{0}F and 14.7 psi is to be heated to 752 ^{0}F and 73.48 psi. The following two options are available: (1) The liquid ethyl benzene is sent through a pump to increase the pressure to the desired value followed by heating it to the required temperature. (2) The liquid ethyl benzene is first vaporized at constant pressure to an intermediate temperature and then compressed to the required pressure. Which of these options do you recommend? Check your answer by simulating both the options using only one flow sheet. (Hint: (1) Use the model Dupl. (2) Use Design Specification to find the intermediate temperature that would give the required temperature of 752 ^{0}F at the exit of the compressor).
5. Simulate to find the heat required to vaporize 45 mol% of a liquid stream entering an evaporator at 50 ^{0}F and 202 psi and containing Propane = 250, n-butane = 400, n-pentane = 350 lbmol/hr. Assume that the evaporator product is at 200 psi.
6. A natural gas stream of 5,000 kmol/hr at 25 ^{0}C and 1500 kPa contains 90% methane, 7% ethane and 3% propane. If the gas is expanded in an isentropic turbine (choose an appropriate pressure) determine the exit temperature and power recovered.
7. Use a simulator to find the minimum number of stages required for a compression system with inter-coolers to compress 600 lb/hr of a mixture of 95mol% hydrogen and 5 mol% methane at 75 ^{0}F and 20 psi to a pressure of 600 psi, if the maximum exit temperature from a compressor stage is 400 ^{0}F. Assume gas outlet temperatures from the intercoolers at 120 ^{0}F.

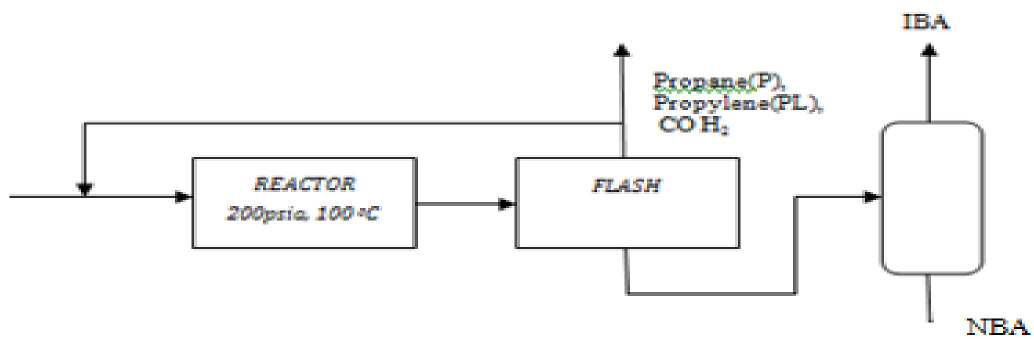
8. Air (15 ^{0}C, 1000 kPa) is mixed with 3000 kg/h of methane at 15 ^{0}C and 1000 kPa. The mixture is then compressed to 2900 kPa and fed to an adiabatic combustor. In the combustor 100%

conversion of methane to CO_2 and H_2O can be assumed. The air flow rate is designed to give a temperature of 1400 ^{0}C at the outlet of the combustor. The hot gas leaving the combustor is expanded in the turbine. Shaft work produced by the turbine is used to power the compressor. Estimate the net rate of power production.

9. Steam at 150 psi and 400 ^{0}F is sent to an expansion turbine with an efficiency of 80%. What is the lowest outlet pressure that can be achieved without condensing any of the steam.
10. A fuel composed of 50% methane and 50% ethane is burned with excess air. The analysis of the flue gas on a dry basis shows 9.00 % CO_2. Simulate to calculate: (a) Percent excess air used (b) the complete Orsat analysis of the flue gases and (c) the moles of flue gas including water vapor / mole of fuel burned. How do you report these answers.
11. A liquid mixture of benzene and toluene with 50wt% of each component is flowing at a rate of 100 gmol/s at 300 K and 1 bar. If heat at a rate of 3600 KJ/s is added, calculate the phase condition and temperature of the exit stream?
12. The feed stock at 1 atm and 298 K consisting of CO (0.5 Kmol/s), H_2 (0.5 Kmol/s), Propylene(PL) 0.47 kmol/s and Propane (P) 0.03 kmol/s is mixed with the recycle stream and enters the reactor. The following reactions take place in the reactor:

$$PL + CO + H2 \rightarrow \text{Isobutyraldehyde (IBA)}$$
$$PL + CO + H2 \rightarrow \text{n-butyraldehyde (NBA)}$$

80% of propylene is converted and the ratio of IBA/NBA = 0.1. The flash column is operating at 0.7 atm and 250K. Assume the last column to give perfect splits for the components shown. Simulate to find the propane flowrate into the reactor when the purge rate changes from 0.1 to 1%.

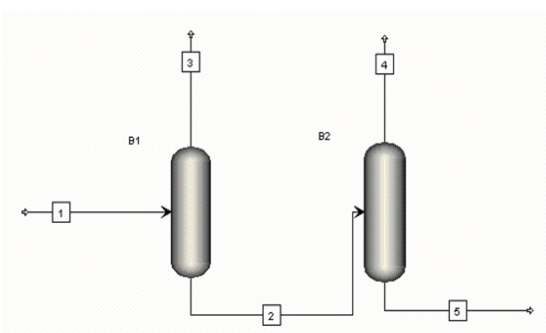


EXERCISE – 6: Columns

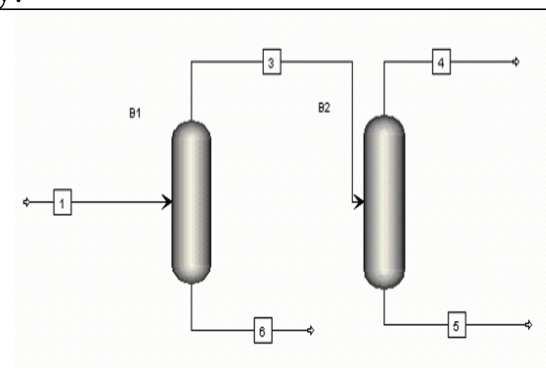
(a) Design a binary distillation column.
Example: Feed consisting of Methanol 36.8%, Water 63.2 mole %.
Feed Flow rate: 120000 lb/hr, Pressure 18 psi, Saturated liquid
Reflux ratio: 1.3 x R_m; Desired recovery of methanol and water in the distillate shall be 98 % and 2% respectively. Perform a sensitivity analysis on the number of stages as a function of reflux ratio in the range 4-15 and plot the results.

(b) Perform Rating calculations using the above design data with Radfrac model.
Design a distillation column for a multi-component mixture and use the data to do rating calculations (Shortcut column followed by Radfrac Column).
Example: The feed consisting of 100 lbmol/h propane, 300 lbmol/h i-butane, 500 lbmol/h n-butane, 400 lbmol/h i-pentane, and 500 lbmol/h n-pentane enters the column at 138 psia and 75^0F. Choose the light and heavy keys as propane and i-butane, the splits desired (99 and 1 percent), the pressure of the column (138 psia), a total condenser. The column operates at 138 psia with a reflux ratio of 10. Simulate using RADFRAC Model and perform sensitivity analysis on the mole fraction of propane in the top product as a function of number of stages.

c) A Mixture of 30% benzene, 25% toluene and 45% ethylbenzene is to be separated by distillation at atmospheric pressure. It is required to obtain three product streams containing almost pure species (say 95% pure) by using two distillation columns in series. Consider the following two schemes: Scheme – A and Scheme – B. In scheme A the more volatile component is with drawn as a top product while in Scheme – B the least volatile component is withdrawn as a bottom product from the first column. Simulate both the schemes under identical conditions and suggest which one of them is better and why?



Scheme – A

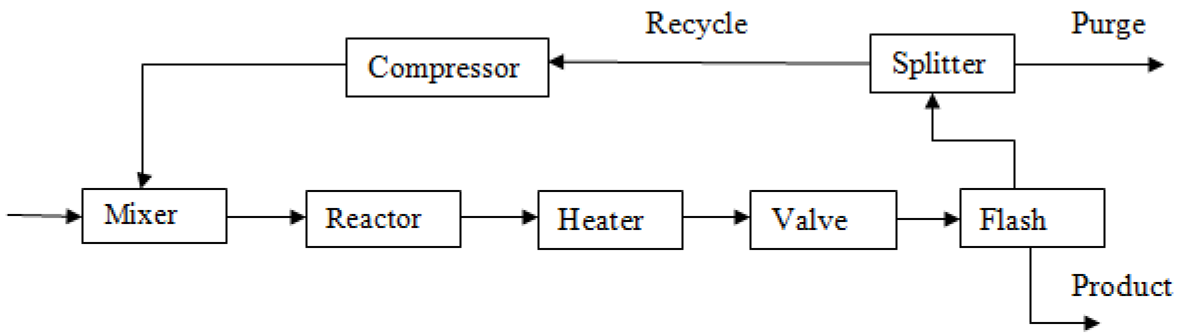


Scheme – B

a) Is your answer going to be valid always?
b) Is your answer going to be valid, if the feed composition is different?
c) Is your answer going to be valid, if the product compositions are different?

EXERCISE – 7

Fresh feed consisting of Propane and propylene is mixed with the recycle stream and enters the reactor. Propylene is converted into 1 hexene in the reactor. The product is separated in the flash column. The unconverted gases are partially purged and the balance recycled. The process flow sheet is as shown below. Simulate the flowsheet using the process data given below:



Process Data:

Feed: 1000 kmol/hr; 150 ^{0}C, 20 bar, Propane: 2%, Propylene: 98%

Reactor: Isothermal at 200 ^{0}C, 20 bar

Reaction: $2C_3H_6 \rightarrow C_6H_{12}$

Fractional conversion = 0.8

Heater: Exit temperature: 120 ^{0}C

Valve: Exit pressure = 12 bar

Flash Column: 120 ^{0}C, 12 bar

Splitter: Purge: 2%

Compressor: Outlet Pressure: 20 bar

a) Keeping the pressure constant, change the temperature in the flash column and observe:
   i) Purity of the product (ii) Product flow rate (iii) Recycle rate (iv) fraction recovery of product

b) Keeping the temperature constant, change the pressure in the flash column and observe:
   i) Purity of the product (ii) Product flow rate
   (iii) Recycle rate (iv) fraction recovery of product

c) List out the product quality, fraction recovery of product and recycle flow rate, at the following conditions of Temperature and Pressure in the flash column: (105, 10); (105, 12); (120,12); (130,12); (140,12).

d) What are the factors that would influence the fraction recovery of Hexene in the liquid product in the flash column?

h) What should be the temperature and pressure in the flash column which would give a product quality of 90 mole % C_6H_{12}.

i) Can you maintain the mole-fraction of propane in the inlet stream to the reactor below 0.05.

EXERCISE – 8

Design Specifications: Use the flowsheet simulated in Exercise – 7.

a) Design Specification: Mole fraction of Hexene in product = 0.85

   In order to meet this requirement vary either the temperature / pressure in the flash column and report the temperature for a given pressure / pressure for a given temperature.

   Alternatively by changing the conversion in the reactor check whether this specification can be met.

b) Design Specification: Inlet temperature to reactor: 200 ^{0}C

   In order to meet this requirement vary the feed temperature and report the temperature of the feed that meets this requirement.

c) Design Specification: 90% of Hexene entering the flash column must be recovered in to the product stream.

   In order to meet this requirement vary the pressure in the flash column and report its value.

d) Design specification: Outlet cooling water temperature can not be more than 10 ^{0}C above the inlet cooling water temperature.

   In order to meet this requirement vary the cooling water flowrate and report its value which meets the specification.

e) Can you use more than one of the above design specifications? If so, try some combinations and report the corresponding results of the manipulated variables along with the specifications.

Sensitivity Analysis:

(a) Perform sensitivity analysis on purity of Hexene in the product as a function of flash temperature at a specific pressure

(b) Perform sensitivity analysis on purity of Hexene in the product as a function of flash Pressure at a specific temperature.

(c) Perform sensitivity analysis on purity of Hexene in the product as a function of both flash temperature and pressure.

(d) Perform sensitivity analysis on Fraction recovery of hexene as a function of pressure in the flash column.

(e) Perform sensitivity analysis on inlet temperature to reactor as a function of feed temperature.

(f) Perform sensitivity analysis on recycle flow rate as a function of temperature / pressure in the flash column

(g) Perform sensitivity analysis on the product flowrate as a function of feed flow rate.

EXERCISE – 9: CALCULATOR BLOCK

Solve the following problems with the help of a calculator block

1. Part of a plant-wide environmental control facility (ECF) is a system for diverting aqueous waste fluids from a discharge point based on the concentration levels of volatile organic compounds (VOCs). If the composition of the VOCs exceed 20 parts per billion, the stream is to be diverted to the second outlet of the splitter. Otherwise, the stream is to be diverted to the first outlet. Test with the two potential feeds listed in the following Table.

Component	VOC	Feed 1 (lb/hr)	Feed 2 (lb/hr)
Methanol	Yes	1	10
Acetone	Yes	2	20
Toluene	Yes	3	30
Methylene chloride	Yes	4	40
Water	No	1.0×10^9	1.0×10^9

2. Ethylidene-Diacetate decomposes on heating to form acetic acid and methyl acrylate:

$$CH_3COOCH(CH_3)COOCH_3 \rightarrow CH3COOH + CH_2{=}CHCOOCH_3$$

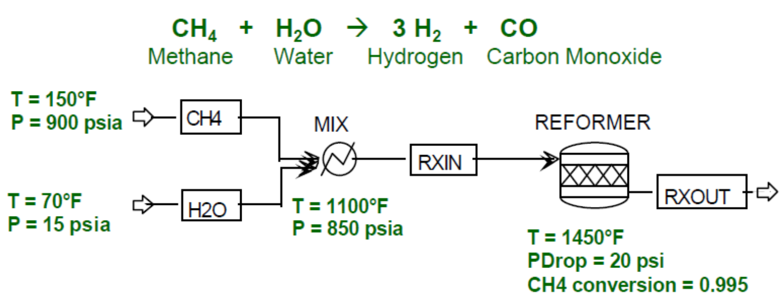
The pyrolysis closely approximates a first-order irreversible reaction with:

$$A = 7.8 \text{ X } 10^9 \text{ and } E = 38{,}200 \text{ cal/mol}$$

Pure reactant enters at a temperature of 800 K and a pressure of 5 atm with a flow rate of 1000 lb/hr. If two perfectly mixed continuous stirred tank reactors of equal volume were to be used in series, what would be the minimum total volume of the two reactors in order to obtain a conversion of 85%.

3. Water at the rate of 1kmol/s is to be heated from 30 ^{0}C to 50 ^{0}C at 5 atm in a heater. Pressure drop (atm) across heater is to be 0.1 x v^2, where v is the volumetric flowrate of water (m^3/s) into the heater. Set up a sensitivity block and report the exit pressure across the heater as the water flowrate in the feed is varied from 1 to 10 kmol/s.

4. Set up a Sensitivity block and report the variation of reactor duty as the methane flowrate in the feed is varied from 100 to 500 lbmol/hr. Note: The methane: water ratio in the reactor inlet must be maintained constant for each sensitivity case at 1: 4.



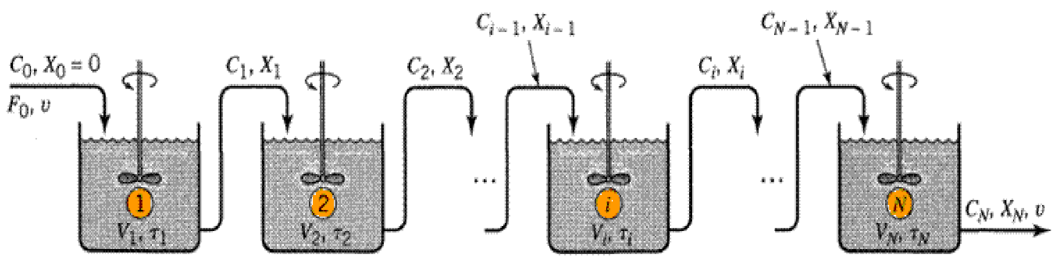
EXERCISE – 10
Optimization

1) A series of four CSTRs operate isothermally at 750K and 1 atm. All the reactors do not have the same volume but the sum of all the four volumes must be equal to 20 m^3. Determine the volumes of the four tanks such that the exit conversion is maximized for an inlet volumetric flow rate of 71 m^3/h. The inlet concentration C_0 = 20 kmol/m^3.

   Ethylidene-Diacetate decomposes on heating to form acetic acid and methyl acrylate:

   $$CH_3COOCH(CH_3)COOCH_3 \rightarrow CH_3COOH + CH_2{=}CHCOOCH_3$$

   The order of the reaction is one with respect to Ethylidene-Diacetate with a rate constant given by: $k = 7.8 \times 10^9 \exp(-38{,}200/RT)$, where T is in K and E in (cal/g mol).

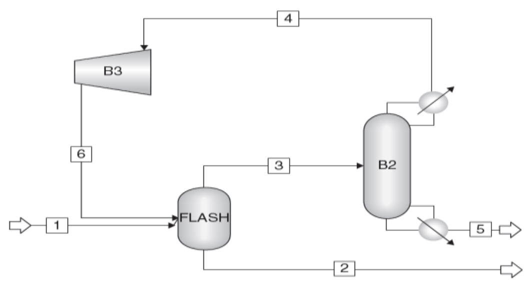


   a) If all the reactors are equal in volume, minimize the total volume of the reactors in order to obtain 50% conversion at the exit of the fourth reactor.

2) A flow rate of 15 m^3/s (q) of air at 50 ^{0}C and a pressure of 1.75 atm is to be compressed to a final pressure of 175 atm. The choice of the type of compressor is influenced by the fact that centrifugal compressors can handle high-volume flow rates but develop low pressure ratios per stage. The reciprocating compressor on the other hand, is suited for low volume flow rates but can develop high pressure ratios. To combine the advantages of each, the compression will be carried out by centrifugal compressor (choose isentropic) in series with a reciprocating compressor (choose positive displacement). The intercooler between the two returns the temperature of the gas to 50 ^{0}C. The equation for costs of compressors are: $C_C = 70\,q + 1600\,P_1/P_0$ and $C_R = 200\,q + 800\,P_2/P_1$, where P_o, P_1 and P_2 are inlet pressures in atm to the centrifugal compressor, reciprocating compressor and final outlet pressure from the reciprocating compressor respectively and q is the inlet volumetric flowrate in m^3/s. Minimize the total cost and report the optimal pressure ratios. Are there any constraint equations in terms of the pressure ratios. Hint: Choose PSRK property method.

3) 5 lbmol/hr of Propane at 14.7 psi and 200 ^{0}F is to be compressed to 120 psi with two single-stage polytropic compressors, using the ASME method, separated by a cooler that reduces the first compressor's outlet temperature to 200 ^{0}F. Develop an optimization that will select the outlet pressure of the first compressor such that the work required for the system is minimized. The polytropic efficiency for both compressors is 0.72 and their mechanical efficiency is 1.0.

4) A key element of the process is the requirement that the column vapor product be compressed to the operating pressure of the flash, which is 150 psi. The flash is to operate adiabatically. The column has 10 theoretical stages with the feed on stage 5. The column reflux ratio is 1.0 and the distillate/feed ratio is 0.5. The overhead product is saturated vapor at a pressure of 50 psi, and the column bottoms pressure is 51 psi. The feed to the process is a saturated liquid at 250 psi and its composition is Propane, 10; n-Butane, 20; n-Pentane, 20; n-hexane, 10 and Cyclohexane, 40 lbmol/hr.



a) Develop an optimization, maximizing profitability, of the flow sheet above by varying the flash pressure between 150 and 250 psi. The objective function needs to incorporate the following terms:

n-hexane value: \$0.1/lbmol
cyclohexane value: \$0.20/mol
Coolant cost: \$1.0 × 10^{-6}/Btu
Heating media cost: \$1.0 × 10^{-7}/Btu
Net work cost: \$0.020/hp

b) Develop an optimization of the flowsheet in three dependent variables. In addition to flash pressure, the column distillate/feed ratio varies between 0.4 and 0.7. The internal reflux ratio varies between 0.4 and 0.7 using the same objective function as above.

EXERCISE – 11: EQUATION ORIENTED APPROACH

Solve all the problems in this exercise using EO approach.
Do not use either sensitivity or design specification tools.

1. 1000 lb/hr of toluene stream (S1) at 100 ^{0}F is mixed with ethylene stream (S2). The flow rate of the ethylene stream which is at 50 ^{0}F is adjusted to achieve the desired temperature of 85 ^{0}F at the mixer effluent. Both the input streams may be assumed to be at a pressure of 1 atm. Simulate the unit and find the flow rate of the stream S2.
2. Benzene at the rate of 50 lbmol/hr is required to be cooled from 100 ^{0}F to 70 ^{0}F. Abundant quantity of cooling water is available at 50 ^{0}F. However, the outlet temperature of the cooling water shall not exceed 65 ^{0}F. Simulate to find the required water flowrate.
3. Determine the volume of a CSTR necessary to produce 300 million pounds of ethylene a year from cracking a feed stream of pure ethane. The reaction is irreversible and elementary. It is required to obtain 60% conversion of ethane, operating the reactor isothermally at 1150K and a pressure of 5 atm.

$$C_2H_6\ (g) \rightarrow C_2H_4\ (g) + H_2\ (g)\ (A \rightarrow B + C)$$

DATA: $k = 0.072 s^{-1}$ at 1000K and Activation Energy, E = 82 kcal/gmol

4. A fuel composed of 50% methane and 50% ethane is burned with excess air. The analysis of the flue gas on a dry basis shows 9.00 % CO_2. Simulate to calculate percent excess air used.
5. The gas phase reversible reaction $C_3H_8 \leftrightarrow C_2H_4 + CH_4$ is allowed to reach equilibrium starting with pure C_3H_8 at a pressure of 1 atm. Simulate to find the temperature at which the reactor must operate in order to obtain a conversion of 80% at equilibrium.
6. Feed consisting of 40%Propane and 60% Isobutane is admitted into a RADFRAC column at 322 K and 20 atm. The feed flowrate is 1 kmol/s. The column has 22 stages. It is required to obtain a propane mole fraction of 0.98 in the top product and a mole fraction of 0.99 with respect to isobutene in the bottom product. The column may be assumed to operate at a pressure of 20 atm. Simulate the column to find the reflux ratio and distillate rate.
7. 50000 kg/hr of a feed consisting of 80% ethylene and 20% ethane at 25 ^{0}C and 25 bar is admitted into a distillation (RADFRAC) column. The column details are: No. of stages: 100, Total condenser, Distillate Rate: 39000kg/hr, Reflux ratio: 4.0 (Mass), Feed Stage: 60. The top stage pressure = 20, Stage 2 pressure = 20.5, the bottom stage pressure = 21.5, feed stage pressure = 21.0. Murphree stage efficiency = 0.9.
   (a) In order to obtain 0.0001 C_2H_6 mole fraction in the distillate and 0.015 C_2H_4 mole fraction in the bottom, calculate the distillate rate and the reflux ratio using EO approach.
   (b) If the selling price of the Distillate and the bottom products are: 0.4 $/kg and 0.1 $/kg, while the cost of condenser duty is 450 $/MMKCal. Optimize the Profit using EO approach that can be obtained as a function of Distillate composition (C_2H_6 mole fraction range: 0.00001 to 0.0002) and bottom product composition (C_2H_4 mole fraction range: 0.001 to 0.05)