BIRLA INSTRITUTE OF TECHNOLOGY & SCIENCE, PILANI, PILANI CAMPUS CHEMICAL ENGINEERING DEPARTMENT

COMPREHENSIVE EXAMINATION

Course Title: Process Design Principles - I Course No.: CHE F314 Marks: 60 Nature of Exam: Closed Book Date: 07/12/2017 Time: 1.5 hrs

Note: Make the suitable assumptions by clearly stating them, if necessary. Write all steps clearly.

1. (4+3+3 = 10 Marks)

BITS institute's canteen requires hot water for its dish-washing. For this purpose, the canteen draws 0.4 kg/s of water at 298 K and heats it to 353 K in a fired-heater. The wastewater leaving the dishwasher is at 333 K. In order to save energy, it is proposed to recover heat from the wastewater to partially heat up the incoming water in a counter-current exchanger as shown schematically below:



Assume that there is no loss of water in the dishwasher and a minimum approach temperature of 10 K should be maintained in the exchanger.

- i. Determine the maximum temperature to which the incoming water can be heated in the exchanger.
- ii. If the overall heat transfer coefficient in the exchanger is 1200 W/m² K and the specific heat capacity of water is 4186 J/kg K, compute the area of the heat exchanger.
- iii. If the cost of the exchanger in 1982 was $2 \times A^{0.41}$ (in lakh rupees), where A is the exchanger area in m² and the Marshall and Swift cost indices in 1982 and 2000 are 315 and 400 respectively, determine the cost of the exchanger in the year 2000.

2. (10 Marks)

One of the major process alternatives for the production of methyl ethyl ketone (MEK) from 2butanol is vapour phase dehydrogenation of 2- butanol. It is a two-step process where 2-butene first hydrated to give 2-butanol. The dehydrogenation of 2-butanol (second-step) is an exothermic reaction which is carried out at 400^oC in presence of Copper, Zinc or Bronze as catalysts. The reactions are as follows:

Step 1:	2-butene + H_2O —		2-butanol
Step 2:	2-butanol —	►	$MEK + H_2$

The reaction products leave the reactor as gas and are split into crude MEK and hydrogen on cooling. The hydrogen is purified by further cooling. The crude MEK is separated from uncreated reactants and by-products by distillation. Unreacted reactants are recycled back to the reactor. We desire to produce 875 mol/hr of MEK. Perform the input-output material balances and calculate the flow rates of unknown streams as a function of design variables.

3. (6 Marks)

A simplified version of process to produce ethylene via ethane cracking has been given by the following reactions:

 $C_2H_6 \rightarrow C_2H_4 + H_2$

 $C_2H_6 \rightarrow 0.5C_2H_4 + CH_4$

Some results for the product distribution are given in the following table.

Table: Product distribution for ethane cracking

Component	Yield Pattern, wt%
H ₂	2.00
CH ₄	1.28
C ₂ H ₄	28.9
C ₂ H ₆	67.8

Estimate the selectivity (moles of C_2H_4 at the reactor exit per mole of C_2H_6 converted) and conversion.

4. (2+2+3+2+3=14 Marks)

Styrene can be produced by following reactions:

Ethylbenzene \Leftrightarrow Styrene + H₂

Ethylbenzene \rightarrow Benzene + Ethylene

Ethylbenzene \rightarrow Toluene + CH₄

The following conditions are given for the above mentioned process:

- a. Reactor temperature and pressure are 1115°F and 25 Psia
- b. The amount produced of H_2 and CH_4 is small.
- c. Boiling points for ethylbenzene 136°C (277°F), styrene 145°C (293°F), Benzene 80.1°C (176.2°F), Toluene 111°C (232°F), Ethylene -103.7°C (-154.7°F), Methane -161 °C (-257.8 °F)

Based on above mentioned conditions, make the following decisions as per conceptual design of process synthesis:

- i. Phase of the reactor effluent (Justification required).
- ii. Do we use phase split? Justify your answer.
- iii. Do we use vapor recovery system?
- iv. Are there any light ends are present? If yes, then what would be the destination?
- v. What should be the liquid recovery system?
- vi. Draw the liquid recovery system and its alternatives for the above process.

5. (20 Marks)

To better understand the similarities and differences between the design of a continuous and a batch process; let us consider a very oversimplified design problem where the process consists of only a single reactor. We desire to produce product B by the reaction $A \rightarrow B$. The cost of A is C_f (\$/mol), we operate 8150 hr/yr for a continuous plant, the desired production rate is *P* mol/hr, the reaction takes place by a first-order isothermal reaction, the separation of the product from unconverted reactants is free, and we cannot recover and recycle any unconverted reactants. We have to pay for the raw materials and reactor, so our cost model becomes:

$$TAC = C_{\rm f} F_F 8150 + C_{\rm v} V$$

The production rate is related to the fresh feed rate FF and the conversion x by the expression

$$P = F_{\rm F} x$$

And the reactor volume is given by:

$$V = \frac{F_{\rm F}}{k\rho_{\rm m}} \ln \frac{1}{1-x}$$

Thus, we can write

$$TAC = \frac{8150C_{f}P}{x} + \frac{C_{v}}{k\rho_{m}x} \ln \frac{1}{1-x}$$

Since the total annual cost becomes unbounded when x approaches either zero or unity, there must be an optimum conversion.

Suppose we do the same process in a batch reactor, where we produce *n* batches per year for 7500 hr/yr. Derive an expression for the total annual cost in terms of the conversion. Let the time it takes to empty, clean, and refill the reactor be t_d and the reaction time per cycle be t_r . How do the expressions for the batch process compare to the result for the continuous plant?

ALL THE BEST

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1. (30 Marks)

For the problem given with minimum approach temperature difference, $\Delta T_{\min} = 20$ °C, carry out the Energy Integration Analysis using Pinch Technology by determining the following:

- (a) Number of heat exchangers based on I law analysis.
- (b) Number of heat exchangers based on II law analysis.
- (c) Hot end design.
- (d) Cold end design.
- (e) Heat exchanger network for the maximum energy recovery (MER).
- (f) Number of loops crossing the pinch.
- (g) Identification of the loops.
- (h) Final heat exchanger network after breaking all independent loops and restoring ΔT_{\min} as and when there is a violation.

Stream No	Condition	FCp (kW/°C)	$h (kW/m^2 °C)$	Source Temperature (°C)	Target Temperature (°C)
1	Hot	40	0.4	180	40
2	Hot	30	0.55	150	60
3	Cold	60	0.75	30	180
4	Cold	20	0.65	80	160

Assume the supply temperature of hot & cold utility are 300 °C and 15 °C respectively. Heat transfer coefficient of hot utility and cold utility is 0.5 kW/m² °C. Pinch temperature is 100 °C (based on hot temperature scale) and the minimum hot and cold utility requirements are 2900 and 600 kW respectively.

2. (30 Marks)

Methanol (CH₃OH) can be produced by the hydrogenation of carbon monoxide in the gas phase as per the reaction:

$CO + 2H_2 \rightarrow CH_3OH$	$\Delta H_{\rm R} = -104.69$ Btu/mol
$CO + 3H_2 \rightarrow CH_4 + H_2O$	$\Delta H_{\rm R} = -198.28 {\rm Btu/mol}$

The reaction takes place at 644 °F and 3500 psia. We desire to produce 100 mol/hr of CH₃OH. Pure carbon monoxide is used as a feed stream, but the hydrogen stream contains 2% of methane. In the recycle stream, composition of carbon monoxide should not exceed by 0.1. The costs of pure carbon monoxide, hydrogen, methane and methanol are 1.0/mol, 1.32/mol, 1.5/mol, and 5.0/mol respectively. Fuel is worth $4.0/10^6$ Btu. Fuel value of carbon monoxide, hydrogen, methane, and methanol are 0.12×10^6 Btu/mol, 0.123×10^6 Btu/mol, 0.383×10^6 Btu/mol, and 0.313×10^6 Btu/mol respectively. Selectivity and conversion relationship is given by:

$$S = 1 - \frac{0.0381}{\left(1 - x\right)^{0.241}}$$

Assume that the reactor cost can be estimated as cylindrical pressurized vessel (CS material) which is having length to diameter ratio as 6.0. Calculate EP₃ in terms of design variables. Forward reaction rate constant is given by:

$$k = 5.88 \times 10^5 \exp\left(\frac{-14,400}{RT}\right)$$

Assume centrifugal compressor (that is $F_c = 1$) for recycle stream; R = 1.987 Btu/mol °R; 1 kWhr = 1.341 bhp; and at STP (32 °F and 14.7 psia), 1 mol of gas occupies 359 ft³ volume. The horse power of compressor can be estimated using:

$$hp = \left(\frac{3.303 \times 10^{-5}}{\gamma}\right) P_{in} Q_{in} \left[\left(\frac{P_{out}}{P_{in}}\right)^{\gamma} - 1\right]$$

where, P_{in} and P_{out} are in lb_f/ft², Q_{in} is in ft³/min, and the values of γ for monoatomic gases, diatomic gases, and more complex gases are 0.40, 0.29, and 0.23 respectively.

Installed compressor cost, $\$ = \frac{840}{280}(517.5)(bhp)^{0.82}(3.11)$

Assume that the compressor and motor efficiencies are 80% and 80% respectively, and the power cost is \$0.045/kWhr.

The Guthrie's correlations for purchased and installed cost of pressurized vessel are given below:

Purchased cost, $\$ = \frac{840}{280} (101.9D^{1.066}H^{0.802}F_c)$

Installed cost, $\$ = \frac{840}{280} 101.9 D^{1.066} H^{0.802} (2.18 + F_c)$

where, D = diameter, ft; H = height, ft; $F_c = F_m F_p$; Fm (correction factor for material) = 1.0

Pressure (psig)	upto 50	100	200	300	400	500	600	700	800	900	1000
Fp	1.00	1.05	1.15	1.20	1.35	1.45	1.60	1.80	1.90	2.30	2.50

ALL THE BEST

SOLUTIONS (CHE F314)

1. Maximum temperature can be achieved by maintaining ΔT_{min} at other end of heat exchanger: Hot stream inlet (333 K) to outlet (308 K). Then cold stream Inlet (298 K) and outlet (T = ?) mCp for both streams are same then mC_r (333 – 308) = mC_r (T – 298) \rightarrow T = 323 K

then
$$mC_p (333 - 308) = mC_p (1 - 298) \rightarrow T = 323 \text{ K}$$

 $Q = mC_p (333 - 308) = 0.4 \times 4186 \times 25 = 41860 \text{ J/sec}$
 $\Delta T_1 = 10 \text{ and } \Delta T_2 = 10$
 $A = \frac{Q}{U\Delta T} = \frac{41860}{1200 \times 10} = 3.488 \text{ m}^2$
 $\text{Cost} = \frac{400}{315} (2)(3.488)^{0.41} = 4.239 \text{ Lakhs}$

2. Input-output structure of the ethylene production process is given below:



The selectivity (S) is defined as the moles of MEK produced to the moles of 2-butene converted.

To produce 875 moles of MEK, number of moles of 2-butene required = 875/S

No. of moles of H_2 formed = 875

No. of moles of H₂O required from fresh feed = 875/S

No. of moles of H₂O in product stream (due to cheaper reactant) = $\frac{875}{S} - 875 = 875 \left(\frac{1-S}{S}\right)$

All input-output flows are the function of selectivity (S).

3. Reactions:

 $C_{2}H_{6} \rightarrow C_{2}H_{4} + H_{2}$ $C_{2}H_{6} \rightarrow 0.5C_{2}H_{4} + CH_{4}$ M.W.: H₂ = 2, CH₄ = 16, C₂H₄ = 28, C₂H₆ = 30 $S = \frac{\text{moles of } C_{2}H_{4} \text{ at the reactor exit}}{\text{moles of } C_{2}H_{6} \text{ converted}}$ Basis: 100 kg of products $n_{H2} = \frac{2}{2} = 1; \quad n_{CH4} = \frac{1.28}{16} = 0.08; \quad n_{C2H4} = \frac{28.9}{28} = 1.032; \quad n_{C2H6} = \frac{67.8}{30} = 2.26$ Moles of C2H6 converted = n_{H2} + n_{CH4} $S = \frac{1.032}{1+0.08} = 0.956$ $x = \frac{1+0.08}{1.08+2.26} = 0.3233$

- i. Vapor. The reactor temperature is 1115°C which is quite high as compare to boiling point of any compound.
- ii. Yes. We can use phase split. However, the amounts of gaseous products are very small so we pass the reactor effluent stream by a condenser and can directly feed to the distillation column for the products separation. But due to the byproduct of ethylene, we may go for phase split.
- iii. No. The amounts of gaseous products (H₂ and CH₄) are very small. However, if we would like to recover ethylene then we have use vapor recovery system.
- iv. Yes. There are two components (H₂ and CH₄) are present as light ends. These components can be burnt in the flair system and heat could be recovered.
- v. Liquid recovery system should be distillation train (sequence of distillation columns).

4.