# CBE 40 Midterm [SOLUTIONS] October 9, 2019 50 minutes

### This exam consists of 3 problems and is worth 100 points.

Write your name and section number (or GSI) on each page! Read each question carefully and follow any instructions given. If any assumptions are necessary, state them AND justify them.

No communication with anyone inside or outside the classroom is permitted. No use of outside materials other than a calculator is permitted.

## Use appropriate significant figures in your answers. Show all work and/or explain your reasoning for full credit. Box your final answers.

On my honor, I have neither given nor received any assistance in taking this exam

Signed:

problem	points	possible points
1	8	35
2	8	35
3	x	30
TOTAL	8	100

Note: -1 point for incorrect sig figs for each occurrence

1. *(35 points)* One growing problem in the realm of chemical engineering is the abundance of ethane from shale gas. A potential use of ethane is to convert it to ethanol for use as a biofuel. To do so, ethane is first converted into ethylene. This reaction produces hydrogen, an important chemical that can be used elsewhere in a refining facility. This is often done in a fluid catalytic cracker unit at 550 °C via the following reaction.

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

Ethylene can then undergo a reaction with water to form ethanol. This reaction is often done at 300 °C and 60 atm in a reactor with phosphoric acid catalyst.

$$C_2H_4 + H_2O \rightarrow C_2H_5OH$$

This stream is then further processed to obtain a nearly pure stream of ethanol. A variety of chemical properties are listed below.

Chemical / Formula / PFD Label	Chemical	Boiling Point	Melting
		(°C)	Point ( $^{\circ}C$ )
Ethane / $C_2H_6$ / Et	Ethane	-89.0	-183
Ethylene / $C_2H_4$ / Ety	Ethylene	-104	-169
Ethanol / $C_2H_5OH$ / EtOH	Ethanol	78.4	-114
Water / $H_2O$ / $H_2O$	Water	100.	0.00
Hydrogen / $H_2$ / $H_2$	Hydrogen	-253	-259

a) Draw a PFD that is capable of converting a stream of pure ethane into ethanol. Be sure to label all reactors and separators with appropriate temperatures. List the components in each stream. You may assume that separations are perfect, but do not assume that reactions go to completion. Assume no reactions occurs other than the two given above. Use recycle streams as much as possible. Use separators to avoid feeding reactor products into a reactor. If you use two or more separators sequentially think about the logical order. You may neglect heat exchangers.

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b) If the conversion of ethylene to ethanol is 85%, how much ethanol can be produced **per year** assuming a feed of 480 mol/hr ethylene?

$$[conversion] = \frac{[(limiting)reactant in] - [(limiting) reactant out]}{[(limiting) reactant in]}$$
$$0.85 = \frac{480 - x}{480}$$

where x is the amount of ethylene exiting the process and (480-x) is the amount of ethylene consumed (or converted to products). Since the problem asks for how much ethanol can be produced, we are interested in (480-x).

[amount of ethylene consumed] = 
$$0.85 * 480 = 408 \left[\frac{mol}{hr}\right]$$

Convert to amount of ethanol produced using stoichiometry:

$$[amount of ethanol generated] = 408 \left[\frac{mol}{hr}\right] * \frac{1 [mol ethanol generated]}{1 [mol ethylene consumed]}$$

$$= 408 \left[\frac{mol}{hr}\right] (ethanol generated)$$

Determine how much can be produced per year:

$$408 \left[\frac{mol}{hr}\right] * \frac{24 \left[hours\right]}{1 \left[day\right]} * \frac{365 \left[days\right]}{1 \left[year\right]} = \mathbf{3.6} \times \mathbf{10^{6}} \left[\frac{mol}{year}\right]$$

- c) How could you increase the conversion of ethylene to ethanol? What would be potential drawbacks of doing so?
  - Recycle more, purge less → Drawback: increased equipment costs to accommodate larger flow rates, increased energy costs for compressing and heating larger amounts

Grading (35 points)

- Part a (20 points)
  - o 6 points isolating ethanol product and H2 product (3 points each)
  - 2 points label reactors with temps
  - 4 points logical separations with temps (1 point each)
  - 3 points including at least 1 recycle stream
    - -1 point if no purge streams
  - $\circ$  3 points label all streams
  - 2 points correct PFD conventions
- Part b (10 points)
  - o 3 points use conversion to find ethylene consumed
  - 3 points Use stoichiometry to find ethanol

- 3 points convert to mol/year
- $\circ$  1 point correct answer
- Part c (5 points)
  - Some effort to discuss recycling more or purging less
  - Other reasonable answer
  - Drawbacks: equipment costs, energy costs, etc.
- 2. *(35 points)* The liquid-liquid absorber below partially absorbs enzyme *E* from an oil solution to a water solution.



#### Absorber specifications:

The oil and water are immiscible; no water dissolves in the oil and no oil dissolves in the water. Streams 2 and 3 leave the absorber in equilibrium. Enzyme *E* preferentially (but *not* completely) dissolves in the water. At equilibrium, the partition of *E* between the oil and water phases is

 $\frac{\text{mass of } E \text{ dissolved in the oil phase}}{\text{mass of oil}} = \frac{1}{1.73} \times \frac{\text{mass of } E \text{ dissolved in the water phase}}{\text{mass of water}}$ 

a) Calculate the flow rates of *E* in streams 2 and 3, in kg/min, using the absorber specifications above.

As given by the problem statement, Streams 2 and 3 leave the absorber in equilibrium, with the equilibrium partition given above. The left-hand side will describe what comes out in Stream 3 and the right-hand side will help determine what comes out in Stream 2. In addition, we know that oil and water are immiscible (no water dissolves in the oil and no oil dissolves in the water). Thus, all water coming into the absorber goes out in Stream 2 and all oil coming into the absorber goes out in Stream 3 (as depicted). The partition equation can be written to suit our problem as such,

$$\frac{F_{3,E}}{115} = \frac{1}{1.73} * \frac{F_{2,E}}{276}$$

We can also write a mass balance of E around the absorber.

Mass Balance of E:

$$F_{1,E} = F_{2,E} + F_{3,E} \implies 1.38 \left[\frac{kg}{min}\right] = F_{2,E} + F_{3,E}$$

Here we have two equations and two unknowns, so the problem is fully specified and we can solve for each of the variables.

$$F_{2,E} = 1.38 - F_{3,E}$$

$$\frac{F_{3,E}}{115} = \frac{1}{1.73} * \frac{1.38 - F_{3,E}}{276}$$

$$(1.73)(276)F_{3,E} = 115(1.38 - F_{3,E})$$

$$(477.48)F_{3,E} = 158.7 - (115)F_{3,E}$$

$$(592.48)F_{3,E} = 158.7$$

$$F_{3,E} = 0.268 \left[\frac{kg}{min}\right]$$

$$F_{2,E} = 1.38 - 0.268 = 1.11 \left[\frac{kg}{min}\right]$$

A second liquid-liquid absorber is added to absorb more E from the oil solution. As before, streams 2 and 3 leave the first absorber in equilibrium. In addition, streams 4 and 5 leave the second absorber in equilibrium. All other absorber specifications are the same as part (a).



b) Calculate the flow rates of E in streams 2 and 5, in kg/min. Note: The flow rates of E in streams 2 and 3 are not necessarily the same as in part (a).

If it wasn't clear as to why Streams 2 and 3 have different flow rates of E compared to part (a), then it should be pointed out that the reason these streams have different flow rates compared to

part (a) is because Stream 4 now has some E which will affect the equilibrium in the first absorber. As such, we can solve this by adopting a similar method as what was done in part (a). First, write out the partition (equilibrium) equations for both absorbers: First absorber:

$$\frac{F_{3,E}}{115} = \frac{1}{1.73} * \frac{F_{2,E}}{276} \tag{1}$$

Second absorber:

$$\frac{F_{5,E}}{115} = \frac{1}{1.73} * \frac{F_{4,E}}{276} \tag{2}$$

It is important to note that the equilibrium equation *only applies to the exit streams* of the absorbers because those are the streams that are in equilibrium!

Then, write out your mass balances for E for each of the two absorbers: First absorber:

$$F_{1,E} + F_{4,E} = F_{2,E} + F_{3,E} \implies 1.38 + F_{4,E} = F_{2,E} + F_{3,E}$$
 (3)

Notice how this equation changed from part (a)! This is what causes the difference in values in Streams 2 and 3 from part (a) to part (b).

Second absorber:

$$F_{3,E} = F_{5,E} + F_{4,E} \tag{4}$$

This time, we have a system of 4 equations and 4 unknowns. The problem is still fully specified, so we can solve for each unknown:

From the first (1) and (2) we have:

1

$$F_{3,E} = \frac{115}{1.73} * \frac{F_{2,E}}{276} = 0.24F_{2,E}$$
(1)

$$F_{4,E} = 1.73(276) \frac{F_{5,E}}{115} = 4.152F_{5,E}$$
(2)

Plugging these into (3) and (4),

$$1.38 + 4.152F_{5,E} = F_{2,E} + 0.24F_{2,E} \tag{3}$$

$$0.24F_{2,E} = F_{5,E} + 4.152F_{5,E} \tag{4}$$

Now we have a system of 2 equations with 2 unknowns.

$$1.38 + 4.152F_{5,E} = 1.24F_{2,E} \tag{3}$$

$$0.24F_{2,E} = 5.152F_{5,E} \tag{4}$$

$$F_{2,E} = 21.5F_{5,E} \tag{4}$$

$$1.38 + 4.152F_{5,E} = 1.24(21.5F_{5,E}) \tag{3}$$

$$1.38 = 22.5F_{5,E} \implies \mathbf{F}_{5,E} = \mathbf{0.0613} \left[ \frac{kg}{min} \right]$$
(3)

$$F_{2,E} = 21.5(0.0613) \Longrightarrow F_{2,E} = 1.32 \left[\frac{kg}{min}\right]$$
 (4)

Grading (35 points)

- Part A (10 points)
  - 4 points use mass balance for overall
  - 4 points correctly use equilibrium equation
  - o 2 points correctly solve system of equations
- Part B (25 points)
  - $\circ$  20 points 5 points for each mass balance/ equilibrium equation
  - o 5 points correctly solving system of equations
- 3. *(30 points)* The feed to an ammonia synthesis process usually contains a small fraction of inert gases, such as argon. These are not condensed and thus are recycled with the unconsumed nitrogen and hydrogen. To avoid a buildup of inerts in the system, which would eventually shut the process down, a purge stream is split off of the recycle stream, as shown in the PFD below:



The following information is known:

- The feed is 100. moles/min and contains 1.00% (molar) inerts and N<sub>2</sub> and H<sub>2</sub> in a **stoichiometric ratio**: 24.75% (molar) N<sub>2</sub>, 74.25% (molar) H<sub>2</sub>.
- The single pass conversion of  $N_2$  (through the reactor alone) is 25.0%.
- The mole percent of inerts in the purge stream is determined to be 12.5%.
- a) Balance the reaction for ammonia synthesis:

$$N_2 + H_2 \rightarrow NH_3$$

Calculate:

- b) the molar flow in the purge stream (Stream 7) per 100 moles/min of fresh feed
- c) the overall conversion of  $N_2$  \_\_\_\_\_\_% (*Hint: Since the fresh feed is in stoichiometric proportions, this proportion of reactants remains the same throughout the process!*)
- d) the total molar flow fed to reactor (Stream 2), including fresh feed and recycle stream

\_\_\_\_\_

(Show your work for full credit; filling in the blanks is not enough! Label flow rates and compositions that you determine on the PFD for maximum partial credit)

#### Solutions:

a) Balance the reaction for ammonia synthesis:

$$N_2 + 3H_2 \rightarrow 2NH_3$$

Calculate:

b) the molar flow in the purge stream per 100 moles of fresh feed: <u>8.00 mol/min /100 mol</u> fresh feed

Calculate using an overall mass balance for the entire system for the inerts:

For the inerts, the mass balance is

$$in = out$$

For a feed of 100 mol, the amount of inerts entering (and exiting) the system according the mass balance is 1%\*100 = 1 mol

We know from the problem statement that in the purge stream, the inerts comprise 12.5%. In other words,

$$x_{feed,I}F_{feed} = x_{purge,I}F_{purge} \Longrightarrow 0.01 * 100 = 0.125 * F_{purge}$$
$$F_{purge} = 8.00 \left[\frac{mol}{min}\right]$$

c) the overall conversion of  $N_2$ \_\_\_92.9 %\_\_\_\_

Since the feed is in stoichiometric proportions, this proportion of reactants remains the same throughout the entire process. In other words, for every mole of  $N_2$  in the purge, recycle, fresh feed, feed to the reactor, and reactor exit, there should be 3 moles of  $H_2$ . Thus, it can be determined that the composition of the purge is as follows:

First, determine the 'remaining' composition of the purge (which comprises N<sub>2</sub> and H<sub>2</sub>):

$$1 - 0.125 = 0.875$$

Then, this percentage should be split into the proportions described above: 1 part  $N_2$ , 3 parts  $H_2$ , for a total of four parts:

$$x_{purge,N_2} = \frac{0.875}{4} = 0.21875$$

$$x_{purge,H_2} = \frac{0.875}{4} * 3 = 0.65625$$

Then, we can calculate the amount of N<sub>2</sub> leaving the process:

$$F_{purge,N_2} = x_{purge,N_2}F_{purge} = 0.21875 * 8 = 1.75 \left[\frac{mol}{min}\right]$$

Finally, use the equation for conversion,

$$[conversion N_2] = \frac{F_{feed,N_2} - F_{purge,N_2}}{F_{feed,N_2}} = \frac{24.75 - 1.75}{24.75} = 92.9\%$$

d) the molar flow fed to the reactor per 100 moles of fresh feed: <u>407 mol/100 mol fresh feed</u> From above, we can see that the amount of N<sub>2</sub> consumed is

$$F_{feed,N_2} - F_{purge,N_2} = 24.75 - 1.75 = 23 \left[ \frac{mol}{min} \right]$$

This means (from stoichiometry) that 46 moles of NH<sub>3</sub> is produced.

$$23 [mol N_2 consumed/min] * \frac{2 [mol NH_3]}{1 [mol N_2]} = 46 [mol NH_3 produced/min]$$

By mass balance, we also know that this amount of  $NH_3$  is what exits the reactor. Since the reactor has a single pass conversion of 25%, this means that 25% of  $N_2$  in the feed of the reactor is converted to products. This means we can find how much  $N_2$  is fed to the reactor. 23 [mol N\_ consumed (min]]

$$F_{reactor feed,N_2} = \frac{23 \left[ mol N_2 \ consumed/min \right]}{0.25} = 92 \left[ mol N_2/min \right]$$

From a mass balance around the combiner, we can find out the amount of N2 in the recycle

$$F_{feed,N_2} + F_{recycle_N_2} = F_{reactor feed,N_2}$$

$$F_{recycle,N_2} = F_{reactor\,feed,N_2} - F_{feed,N_2} \implies F_{recycle,N_2} = 92 - 24.75 = 67.25 \left[\frac{mol}{min}\right]$$

We know the composition of the recycle stream (same as purge since compositions are preserved around a splitter), so we can find the total recycle amount:

$$F_{recycle} = \frac{F_{recycle,N_2}}{x_{recycle_{N_2}}} = \frac{67.25}{0.21875} = 307 \left[\frac{mol}{min}\right]$$

Finally, by mass balance, the feed to the reactor can be found:

$$F_{reactor feed} = F_{feed} + F_{recycle} = 100 + 307 = 407 \left[\frac{mol}{min}\right]$$

Grading (30 points)

- Part A (5 points)
  - $\circ$  All or nothing
- Part B (5 points)
  - o 4 points Using overall mass balance on inert
  - $\circ$  1 point correct answer
- Part C (10 points)
  - 2 points determine purge composition

- $\circ \quad 2 \text{ points} \text{recognizing ratio from } N_2 \text{ to } H_2 \text{ is consistent}$
- $\circ$  3 points N<sub>2</sub> leaving process
- $\circ$  3 points conversion equation
- Part D (10 points)
  - $\circ$  1 point stoichiometry N<sub>2</sub> NH<sub>3</sub>
  - $\circ$  3 points mass balance reactor (N<sub>2</sub>)
  - o 2 points mass balance combiner
  - 0 1 point splitter composition preserved
  - o 2 points solve recycle stream
  - 0 1 point correct value for reactor feed