

**PRAIRIE VIEW A&M UNIVERSITY
ROY G. PERRY COLLEGE OF ENGINEERING
DEPARTMENT OF CHEMICAL ENGINEERING
CHEG 3305 SEPARATION PROCESS, SPRING 2022**

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Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

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Original Homework Questions & Master Solution/grading scheme used

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

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Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

Course Description in ABET Format

I. COURSE DESCRIPTION IN ABET FORMAT

COURSE SYLLABUS

CHEMICAL ENGINEERING DEPARTMENT

CHEG 3305 P02 Separation Processes

1.	Course number and name:	CHEG 3305 Separation Processes
2.	Credits, contact hours, categorization:	3 credit hours; 5 contact hours; engineering
3.	Instructor's or course coordinator's name:	Dr. Nabila Shamim
4.	Text book: Title:	Transport Processes and Separation Process Principles. 5th Edition, ISBN: 0-13-101367-X
	Author:	Geankoplis, C.J.,
	Publisher, Year & Edition:	Prentice-Hall, (5th Edition).
	a. Other Supplemental material	Unit Operations of Chemical Engineers. 7th Edition, McCabe, Smith and Harriott, McGraw-Hill, 2005 ISBN: 9780073104454
5.	Specific course information	
	a. Brief description of the content of the course (catalog description)	(3-0) Credit 3 semester hours. Applications of heat and mass balances and phase equilibria to the design of staged separation processes. Use of graphical methods such as McCabe Thiele. Application to distillation, absorption, stripping, and extraction Goals: The goal of this course is to teach students the science and design of separation processes.
	b. Prerequisites or Co-requisites	CHEG 2304 (CHEG 2043) and CHEG 3304 (CHEG 3053)
	c. *Indicate whether a required, elective, or selected elective (as per definition provided) course in the program	Required
6.	Specific goals for the course	Students will be able to:
	a. specific outcomes of instruction	1. Solve for an unknown process variable using general algebra and linear algebra techniques. 2. Apply calculus and differential equation principles when determining diffusion. 3. Interpret and construct graphs and tables such as a triangle plot and calculating area under a curve. 4. Write and reduce mass balance equations around trays, stages, or overall processes. 5. Write and reduce energy balance equations around trays, stages, or overall processes. 6. Identify the phases present and select an appropriate

		method of separation. 7. Depict a process in a flow diagram labeling unknown and known quantities. 8. Utilize Henry's and Raoult's laws to determine vapor and liquid composition. 9. Calculate compositions for single stage and multiple stage systems using Fenske equation. 10. Calculate mass fluxes, molar fluxes, and overall fluxes using correct formulas. 11. Calculate tower heights, number of trays, and efficiency using correct formulas. 12. Simulate separation processes using computer software such as Aspen/HYSYS. 13. Plot equilibrium data and operating lines on an XY plot and determine the number of stages/trays and the feed location. 14. Discuss simulation results and recommendations in memos and reports.
	b. Explicitly indicate which of the student outcomes listed in Criterion 3 or any other outcomes are addressed by the course.	This course addresses: Course Outcome 1: Ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics 1. Identify and Formulate engineering/technical/computing problems using principles of engineering/mathematics/science 2. Solve CEP/computing problems.
7	Brief list of topics to be covered	1. Mass Transfer and Diffusivity (6 hours) 2. Evaporation (3 hours) 3. Contact Stages (3 hours) 4. Absorption (6 hours) 5. Humidification and Drying (6 hours) 6. Distillation (9 hours) 7. Leaching/Extraction (6 hours) 8. Design using Aspen/HYSYS (6 hours)

Prepared by: Dr. Nabila Shamim

Date: May 20, 2022

II ASSESSMENT RESULTS FOR CURRENT AND PAST THREE PERIODS

Program Outcomes Assessed in this course

Outcome 1:

An ability to identify, formulate, and solve complex engineering problems (CEP) by applying principles of engineering, science, and mathematics.

Assessment Summary of Class Semester Averages for Outcomes (Should be provided for Fall 2019 through Spring 2022 Assessment Period)

Outcomes	1
Semester	Semester Class Average (%)
Spring 2022	81
Spring 2021	75
Spring 2020	72.4
Spring 2019	64
Comments on Trend of Data (Improving or deteriorating)	The average for this outcome shows gradual increase from class average 64 in the Spring 2019 to 81 in the Spring 2022

*Expected Semester Class Average = 70% (or as defined by the program)
Ideal Semester Class Average = 75% (or as defined by the program)

End of Semester Course Assessment Reports Spring 2022 and Last Three Assessment Periods.

Each summary contains the following Information

1. Performance Statistics

- Total number of students in class
- The class average performance (**stated as %**) in each course outcome assessed in this class and the **two previous times course was assessed**.
- The acceptable class average for the class in each outcome area as set by your Department.
- Percentage of students who scored below the expected average in each outcome.

2. Implementation Summary

- Brief summary of plans implemented during the semester based on last assessment report

3. Perceived Problems

- Instructor's **critical evaluation** of perceived problems that affected students' performance. **Realistic problems should be identified throughout the semester and summarized in this section of the report.**

4. New Plans for Addressing Problems

- Instructor's plans for addressing the perceived problems the next time the class is taught. **These should be specific enough for another instructor to implement. Most of these should be things that, you, the instructor can implement to help students to improve. Be creative.**

5. Overall Trend over last three assessment periods

- Instructors summary of overall performance trend for each outcome measured over the last three periods.

5. Were Expectations Met?

- Answer **YES** if the **class average was above the expected average** and the **stated percentage of students** scored at or above the expected average, else answer **NO**.

Table 2.1 END OF SEMESTER COURSE OUTCOME ASSESSMENT REPORT
CHEG 3305 SEPARATION PRCESS: SRPING 2021 SEMESTER
Report Prepared by: Dr. NABILA SHAMIM Report Date: May 18, 2022

Report Prepared by: Dr. Brijesh Kumar Singh Report Date: May 18, 2022														
Semester	Analysis Type	Number of Students	Outcome 1.1 Ability to identify and formulate Separation problems using the principles of mathematics, engineering, and science.				Outcome 1.2 Absorption and distillation problems using computing tools.				Outcome 1 Ability to identify and formulate problems using the principles of mathematics, engineering, and science.			
			Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average
Spring 2022	Direct	20	75	70	74	55	75	70	89	100	75	70	81	75
Spring 2021	Hybrid	30	75	70	72	57	75	70	78	80	75	70	75	67
Spring 2020	Direct	30	75	70	69	60	75	70	84	96	75	70	76.6	72.4
Spring 2019	Direct	33									75	70	75	64
Implementation Summary	Items implemented from previous report or after meeting previous instructor		- the following techniques and technologies were included: 1. Students were divided into small groups with a specific problem to Think-Pair-Share. 2. Discussion topics were assigned in CANVAS to shared thoughts with instructor, peers and made comments. Technology used: Surface pro is used to deliver online lectures. OneNote software gave the opportunity to write the lecture topics on white page and simultaneously share with students. - The split screen option is a game changer, it gave the privilege to share the theory and solve the problem side by side. - Used active learning and collaboration tools to make the class more interactive,. - Individually students were assessed using exams and quizzes.				- The importance of the use of HYSIS/ASPEN in engineering practice was stressed at the middle of the course. - Complex assignments were given in groups based on technical issues students use ASPEN to solve. - A detail rubric on the project Aspen HYSYS tutorial was given to students. In CHEG 3305 the number of Aspen assignments were increased for students to get more familiar with process simulation. A SOP was provided showing the steps to get remote access. However, due to license issue they could not complete three projects - A detailed SOP shared with student to complete ASPEN HYSYS project on distillation unit.				Students learned in detail about different separation units. Pressure drop and temperature variation in column			
Perceived Problems	Perceived problems are directly related to the PC and the sub items under them		Students had trouble formulating the material and energy balance equation and basic mass transfer theorems for example				- Students just presented graphs from simulation; explanation was not clear - Students are not ready to				Problems were mentioned in the sub-outcomes.			

		Rault's law, Fick's law. • Instructor get overwhelmed with grading • Not all students were focused during the class	work hard. • Due to pandemic academic integrity was at risk.	
Plans for Addressing Problems	Plans for address specific measures to address PC and their sub areas	The following is recommended for implementation. • Teaching assistance is needed to support instructor. • The instructor should do more active learning in class and give assignments collaborative learning.	TA is needed to support instructor. One day workshop on ASPEN HYSYS will help students complete projects	Plans to address problems mentioned in the sub-outcomes
Overall Trend over Periods	Ascertain if there were improvements over previous semesters	Class average and the percentage of students reaching the expected outcome did not meet requirements.	Students' performance met the expected class average.	Students' performance met the expected class average
Were Expectations Met?	Class Average $\geq 75\%$ and $\geq 70\%$ of Students Performed at or Above Expected Average.	NO	YES	YES

Table 2.1 END OF SEMESTER COURSE OUTCOME ASSESSMENT REPORT
CHEG 3043 SEPARATION PROCESS: SPRING 2020 SEMESTER
Report Prepared by: Dr. NABILA SHAMIM Report Date: May 18, 2020

Semester	Analysis Type	Number of Students	Outcome 1.1 Ability to identify and formulate Separation problems using the principles of mathematics, engineering, and science.				Outcome 1.2 Ability to solve complex Absorption and distillation problems using computing tools.				Outcome 1 Ability to identify and formulate problems using the principles of mathematics, engineering, and science.			
			Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average
Spring 2020	Direct	30	75	70	69	60	75	70	84	96	75	70	76.6	72.4
Spring 2019	Direct	33									75	70	75	64
Implementation Summary	Items implemented from previous report or after meeting previous instructor		2. Students worked on identifying and formulating problems in groups 3. Individually students were assessed using exams and quizzes.				The importance of the use of HYSIS/ASPEN in engineering practice was stressed at the middle of the course. Tutorial class were taken to familiarize student with HYSIS. Complex assignments were given in groups based on technical issues students use ASPEN to solve. A detail rubric on the project Instructor made necessary arrangements to access software remotely				Students learned in detail about different separation units. Pressure drop and temperature variation in column			
Perceived Problems	Perceived problems are directly related to the PC and the sub items under them		Students had trouble formulating the material and energy balance equation and basic mass transfer theorems for example Rault's law, Fick's law.				Students worked as a group to finish the assignments however there was lack of team effort. Students just presented graphs from simulation; explanation was not clear				Problems were mentioned in the sub-outcomes.			
Plans for Addressing Problems	Plans for address specific measures to address PC and their sub areas		The following is recommended for implementation. The instructor should do more active learning in class and give assignments collaborative learning.				The instructor should: Continue providing handouts detailing effective use of Excel spreadsheet and HYSYS and how to explain data.				Plans to address problems mentioned in the sub-outcomes			
Overall Trend over Periods	Ascertain if there were improvements over previous semesters		Class average and the percentage of students reaching the expected outcome did not meet requirements.				Students' performance met the expected class average.				The class average was same as before and expected outcome were significantly higher than the previous year.			
Were Expectations Met?	Class Average $\geq 75\%$ and $\geq 70\%$ of Students Performed at or Above Expected Average.		NO				YES				NO			

CHEG 3305 SEPARATION PROCESSES, SPRING 2022

Title of Assignment: Exam 1

TOPICS COVERED IN Exam 1

Test 1 covered the following topics:

1. Solving complex problems on Absorption and Diffusion process
 - a. General balance equation
 - b. Calculate number of stages

CHEG 3305 SEPARATION PROCESSES, SPRING 2022

**SAMPLE TEST QUESTIONS, SOLUTION,
AND GRADING SCHEME FOR MID-TERM EXAM**

Separation Processes CHEG 3305 P02 (Spring 2022)

Exam 1 Time: 2 Hrs Date: March 7 2022

Total points: 100

STUDENT NAME:DATE:

**Closed Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO RESTROOM
BREAKS NO COLLABORATION**

PROVIDE UNITS ON ALL CALCULATIONS AND ANSWERS

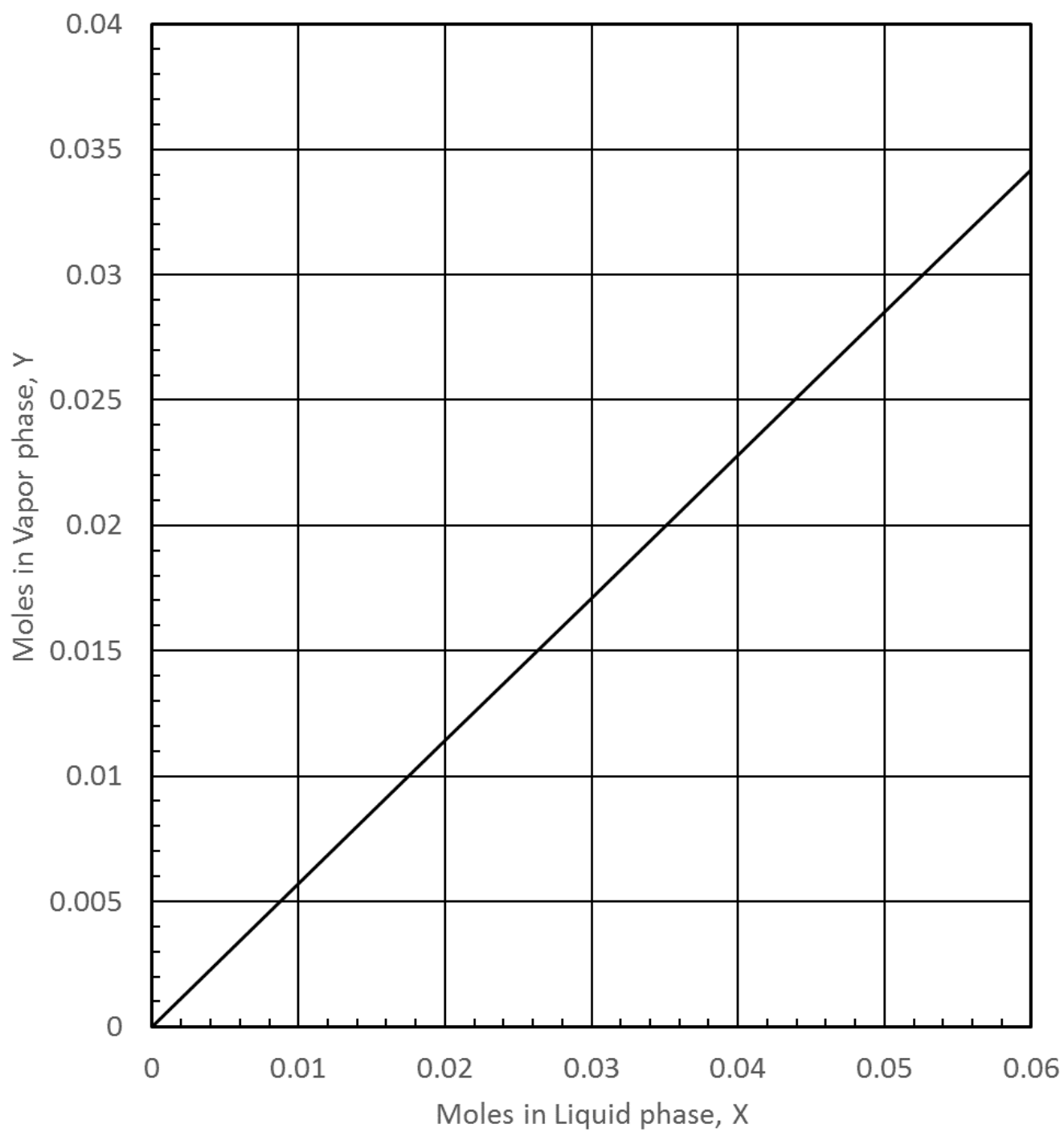
ANY DISHONESTY DURING THE EXAM WILL RESULT IN “F” GRADE

WORK ALL PROBLEMS ON THE QUESTION SHEETS AND DO NOT USE ANY SHEET
OF YOUR OWN

Student Signature:

Problem 1 (40 Points) Molasses is fermented to produce a liquor containing ethyl alcohol. The CO_2 rich vapor containing a small amount of ethyl alcohol enters the column at 180 kmol/h at 30°C and 110 kPa, which contains 97% CO_2 and 3 % ethyl alcohol. The alcohol can be recovered by absorption with pure water in a sieve tray tower. During the absorption process 98% ethyl alcohol is absorbed. The liquid flow rate (actual solute free absorbent) is 50% above the minimum liquid rate. The equilibrium relationship is $Y^* = 0.57 X$.

- a. Draw a schematic diagram of the absorption column and label it clearly showing all given information and unknown. (5 Points)
- b. Clearly Write the assumptions of McCabe-Thiele Method (5 Points)
- c. Determine the mole fraction of ethyl alcohol at the top of the column (7 Points)
- d. Calculate the pure water flow rate used to absorb ethyl alcohol. (8 Points)
- e. Determine the mole fraction of ethyl alcohol in water at the bottom of column (5 Points)
- f. Use McCabe Thiele Method to graphically calculate the theoretical number of stages (10 Points)



Problem 2 (20 Points 2 Points each)

- a) For the determination of driving force in any mass transfer operation, the solubility of a species in a solvent, i.e., equilibrium distribution between phases is important. With the increase in temperature, solubility of a gas in liquid increases. Hence, absorption is done at higher temperature. On the contrary, desorption is done at lower temperature. (True/False)
- b) Diffusivity in gas is proportional to $1/\mu$ (True/False)
- c) Which of the following is NOT true of diffusion in gases, liquids and solids?
- The rate of diffusion depends on the component diffusing; the medium is not very important
 - The rates of diffusion in liquids and gases is different by several orders of magnitude
 - The rates of diffusion in liquids and solids is different by several orders of magnitude
 - The rate of diffusion in solids and the rate of diffusion in liquids are both slower than in gases
- d) Mass transfer is driven by concentration gradient as well as by pressure gradient and electrical gradient. (True/ False)

Answer the following two questions using the plot below (2points each)

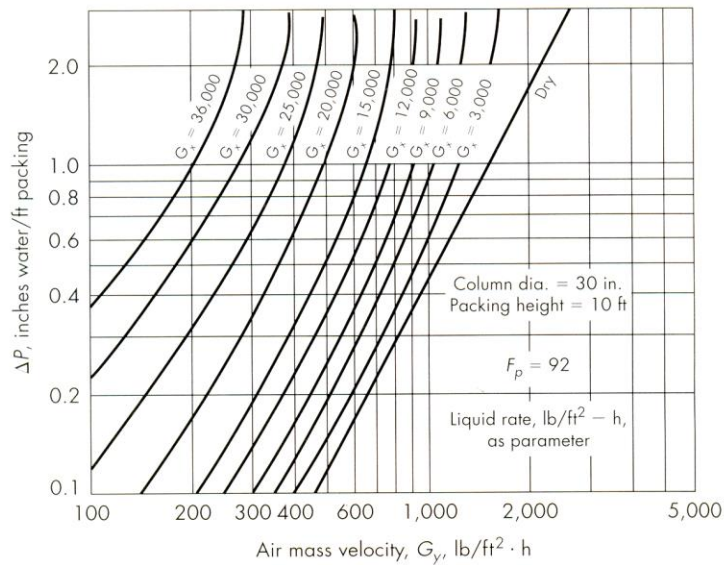
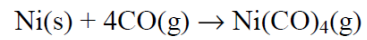


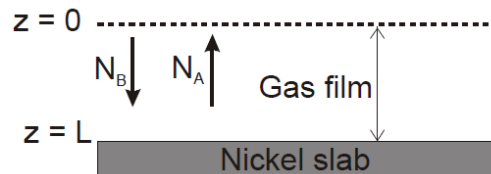
FIGURE 18.4
Pressure drop in a packed tower for air-water system with 1-in. Intalox saddles. (1,000 lb/ft²·h = 1.356 kg/m²·s; 1 in. H₂O/ft = 817 Pa/m)

- e. At very low liquid rates, the effective cross section of the packing is not appreciably different from that of dry packing and pressure drop is due to flow through a series of variable openings in the bed that is called channeling. (True / False)
- f. From the above figure write down what is the pressure drop when flooding takes place..... (fill in the blank)
- g. Factors that may lead to flooding:
 - a. High inlet gas flow rates
 - b. Low liquid circulation rates
 - c. Small diameter towers
 - d. All of the above
- h. The process of the purification of natural gas by contact with an ethanolamine (alkaline) solution is called absorption (True /False)
- i. Write only the general equation for diffusion of gases A and B

Problem 3 (a-d) (40 points) Nickel carbonyl (A) is produced by passing carbon monoxide (B) at 350 K and 1 atm over a nickel slab. The following reaction takes place at the solid surface:



The reaction is very rapid, so that the partial pressure of CO at the metal surface is essentially zero. The gases diffuse through a film with a thickness $L = 0.7$ mm.



Ability of Identify Engineering Problem

a. List all the assumptions; simplify the general mass transfer equation for species A.

(5 Points)

- b. Draw a schematic diagram of the concentration profile for the given system and specify your boundary conditions. **(10 Points)**

Ability of Formulate Engineering Problem

- c. Develop the final integrated equation for the flux of species B; be sure to use your boundary conditions. **(15 Points)**

Ability of solve Engineering Problem

- d. Estimate the rate of production of nickel carbonyl (A), in mole/s $\cdot$ cm² of solid surface at steady state. The composition of the bulk gas phase ($z = 0$) is 35 mol% CO. The binary diffusivity is $D_{AB} = 20.0$ mm²/s. **(10 Points)**

ABOVE AVERAGE

Above Average Student Original Graded Assignment

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Separation Process CHEG 3305 P02 (Spring 2022)

Exam 1 Time: 2 Hrs Date: March 7 2022

Total points: 100

STUDENT NAME: *93 Excellent* Vivian Patthammavong DATE: *03/07/2022*

**Closed Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO RESTROOM
BREAKS NO COLLABORATION**

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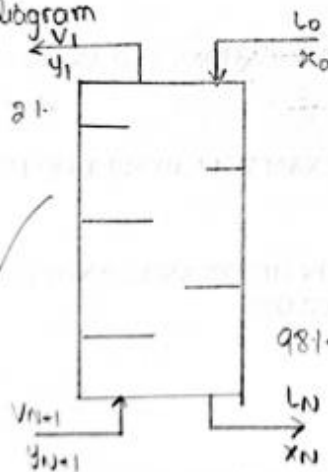
**WORK ALL PROBLEMS ON THE QUESTION SHEETS AND DO NOT USE ANY SHEET
OF YOUR OWN**

Student Signature: *Vivian*

Problem 1 (40 Points) Molasses is fermented to produce a liquor containing ethyl alcohol. The CO_2 rich vapor containing a small amount of ethyl alcohol enters the column at 180 kmol/h at 30°C and 110 kPa , which contains $97\% \text{ CO}_2$ and $3\% \text{ ethyl alcohol}$. The alcohol can be recovered by absorption with pure water in a sieve tray tower. During the absorption process 98% ethyl alcohol is absorbed. The liquid flow rate (actual solute free absorbent) is 50% above the minimum liquid rate. The equilibrium relationship is $Y^* = 0.57 X$.

- Draw a schematic diagram of the absorption column and label it clearly showing all given information and unknown. (5 Points)
- Clearly Write the assumptions of McCabe-Thiele Method (5 Points)
- Determine the mole fraction of ethyl alcohol at the top of the column (7 Points)
- Calculate the pure water flow rate used to absorb ethyl alcohol. (8 Points)
- Determine the mole fraction of ethyl alcohol in water at the bottom of column (5 Points)
- Use McCabe Thiele Method to graphically calculate the theoretical number of stages (10 Points)

② Draw a diagram



given: $Y^* = 0.57 X$

$$V_{n+1} = 180 \text{ kmol/h}$$

$$y_{n+1} = 0.03$$

$$T = 30^\circ\text{C}, P = 110 \text{ kPa}$$

absorb 98% .

$$(50\%) L_{\min} = (98 + 0.5) = 98.5 \text{ kmol/h}$$

$$x_0 = 0$$

98% absorbed

$$\frac{L}{V} = 1.5 \left(\frac{L}{V} \right)_{\min}$$

$$-3$$

③ assumption

- Solvent is non-volatile
- Carrier gas is insoluble
- System are isobaric and isothermal
- The heat absorption is negligible

$$\begin{aligned} \# \text{ amount of ethyl alcohol entering} &= (V_{n+1})(y_{n+1}) \\ &= (180 \text{ kmol/h})(0.03) \\ &= 5.4 \text{ kmol/h} \end{aligned}$$

$$\begin{aligned} \# \text{ amount of } CO_2 \text{ entering} &: (1 - y_{n+1}) V_{n+1} \\ &= (1 - 0.03)(180) \\ &= 174.6 \text{ kmol/h} \checkmark \end{aligned}$$

$$\begin{aligned} \# \text{ ethyl alcohol leaving in } V_1(2.1) &= (0.02)(5.4) \\ &= 0.108 \text{ kmol/hr} \checkmark \end{aligned}$$

$$\Rightarrow V_1 = CO_2 \text{ entering} + \text{ethyl alcohol leaving}$$

$$V_1 = (0.108 + 174.6) \text{ kmol/h}$$

$$V_1 = 174.708 \text{ kmol/h} \checkmark$$

$$\Rightarrow y_1 = \frac{0.108 \text{ kmol/h}}{174.708 \text{ kmol/h}} = 0.00062 \checkmark$$

$$\begin{aligned} \# \text{ Liquid entering} &= (1.5)(98 + 0.5) \\ L_0 &= 147.75 \text{ kmol/h} \end{aligned}$$

check calculation.

$$\begin{aligned} \# \text{ amount of ethyl alcohol leaving in } L_N(98.1) & \\ (0.98)(5.4) &= 5.292 \text{ kmol/h} \end{aligned}$$

$$\Rightarrow L_N = 5.292 \text{ kmol/h} + 147.75 \text{ kmol/h}$$

$$L_N = 153.042 \text{ kmol/h} \checkmark$$

$$\Rightarrow x_N = \frac{5.292 \text{ kmol/h}}{153.042 \text{ kmol/h}} = 0.035 \checkmark$$

$$A_1 = \frac{L_0}{mV_1} = \frac{147.75}{(0.57)(174.708)} = 1.48$$

$$A_N = \frac{L_N}{mV_{N+1}} = \frac{153.042}{(0.57)(180)} = 1.49$$

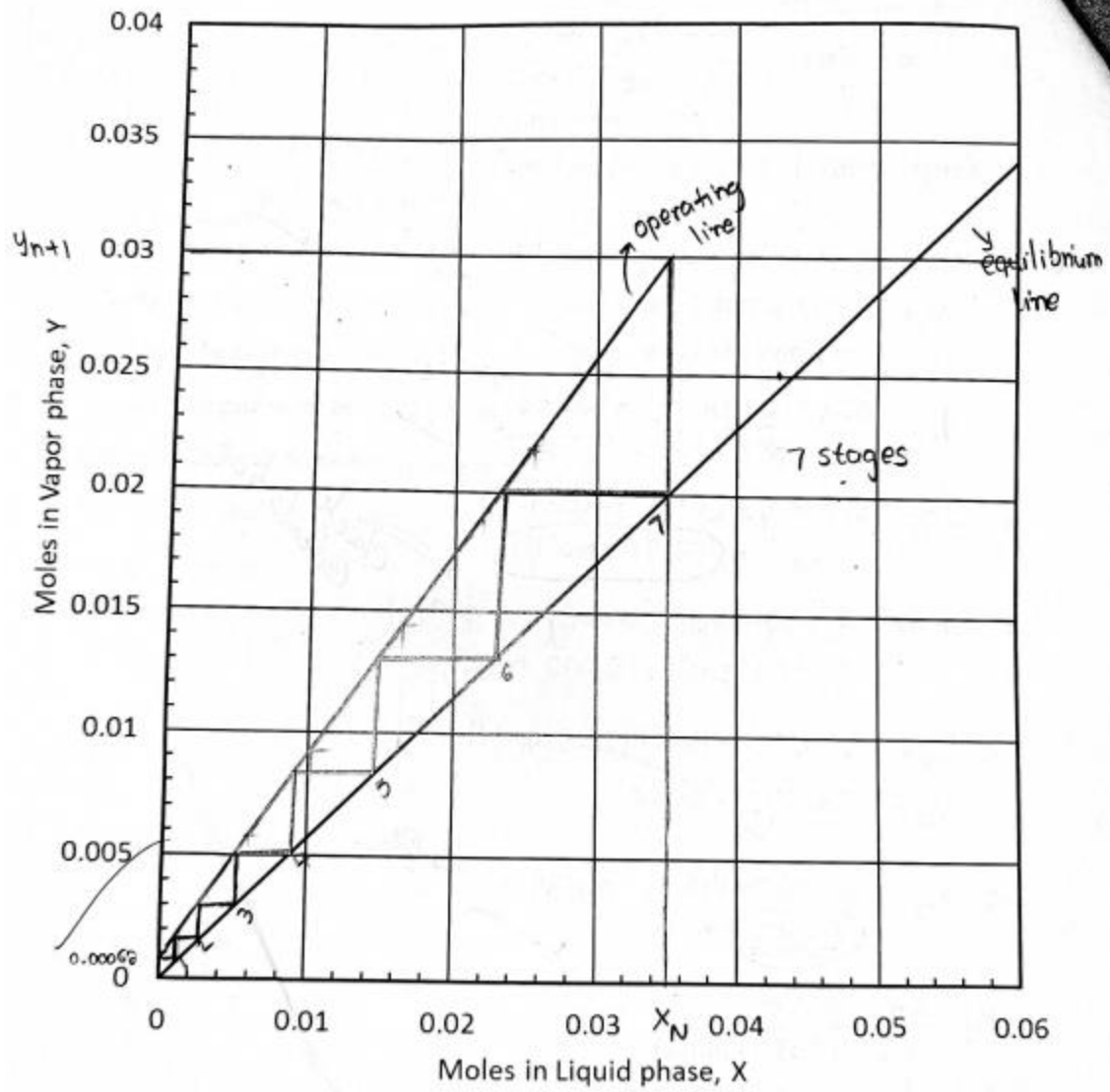
$$A = \sqrt{(1.48)(1.49)} = 1.48$$

$$N = \frac{\ln \left[\frac{y_{n+1} - mx_0}{y_1 - mx_0} \left(1 - \frac{1}{A} \right) + \frac{1}{A} \right]}{\ln A}$$

$$N = \frac{\ln \left[\frac{0.03 - 0}{0.00062 - 0} \left(1 - \frac{1}{1.49} \right) + \frac{1}{1.49} \right]}{\ln 1.49} = 7 \text{ stages}$$

$$(x_0, y_1); (x_N, y_{n+1})$$

$$(0, 0.00062); (0.035, 0.03)$$



Problem 2 (20 Points 2 Points each)

- a) For the determination of driving force in any mass transfer operation, the solubility of a species in a solvent, i.e., equilibrium distribution between phases is important. With the increase in temperature, solubility of a gas in liquid increases. Hence, absorption is done at higher temperature. On the contrary, desorption is done at lower temperature. (True/False) **(False)**
- b) Diffusivity in gas is proportional to $1/\mu$ (True/False) **(True)**
- c) Which of the following is NOT true of diffusion in gases, liquids and solids?
- The rate of diffusion depends on the component diffusing; the medium is not very important
 - The rates of diffusion in liquids and gases is different by several orders of magnitude
 - The rates of diffusion in liquids and solids is different by several orders of magnitude
 - The rate of diffusion in solids and the rate of diffusion in liquids are both slower than in gases
- d) Mass transfer is driven by concentration gradient as well as by pressure gradient and electrical gradient. (True/False) **(True)**

Answer the following two questions using the plot below (2points each)

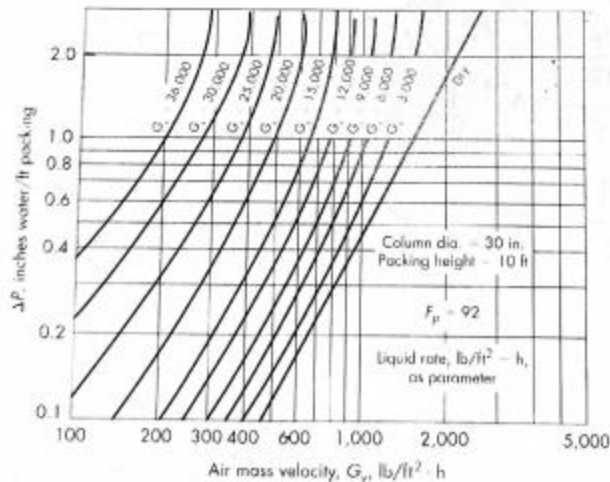


FIGURE 18.4
Pressure drop in a packed tower for air-water system with 1-in. Intalox saddles. ($1,000 \text{ lb/ft}^2 \cdot \text{h} = 1.356 \text{ kg/m}^2 \cdot \text{s}$; 1 in. $\text{H}_2\text{O}/\text{ft} = 817 \text{ Pa/m}$)

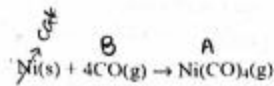
- e. At very low liquid rates, the effective cross section of the packing is not appreciably different from that of dry packing and pressure drop is due to flow through a series of variable openings in the bed that is called channeling. (True/False)
- f. From the above figure write down what is the pressure drop when flooding takes place. ΔP_F (fill in the blank)
- g. Factors that may lead to flooding:
- High inlet gas flow rates
 - Low liquid circulation rates
 - Small diameter towers
 - ☒ All of the above
- h. ☒ The process of the purification of natural gas by contact with an ethanolamine (alkaline) solution is called absorption. (True/False)
- i. Write only the general equation for diffusion of gases A and B

$$N_A = -D_{AB} \frac{dc_A}{dz} + \frac{c_A}{c_T} (N_A + N_B)$$

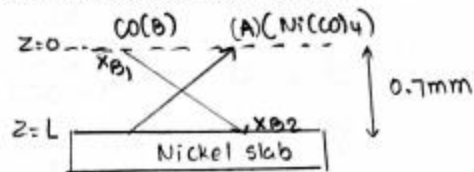
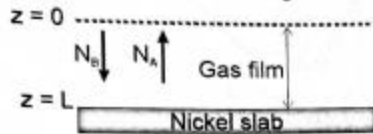
$$N_A = -\frac{D_{AB}}{RT} \frac{dp_A}{dz} + \frac{p_A}{p_T} (N_A + N_B)$$

$$N_A = -CD_{AB} \frac{dx_A}{dz} + x_A (N_A + N_B)$$

Problem 3 (a-d) (40 points) Nickel carbonyl (A) is produced by passing carbon monoxide (B) at 350 K and 1 atm over a nickel slab. The following reaction takes place at the solid surface:



The reaction is very rapid, so that the partial pressure of CO at the metal surface is essentially zero. The gases diffuse through a film with a thickness $L = 0.7$ mm.



Ability to Identify Engineering Problem

a. List all the assumptions; simplify the general mass transfer equation for species A.

- assumption
- Steady state
 - Heterogeneous chemical reaction
 - Instantaneous surface reaction



$$\frac{r_B}{-4} = \frac{r_A}{1}$$

$$\frac{N_B}{-4} = N_A \Rightarrow N_B = -4N_A$$

(5 Points)

$$N_A = -CD_{AB} \frac{dx_A}{dz} + x_A(N_A + N_B)$$

$$= -CD_{AB} \frac{dx_A}{dz} + x_A(N_A - 4N_A)$$

$$N_A = -CD_{AB} \frac{dx_A}{dz} - 3N_A x_A$$

$$N_A(1 + 3x_A) = -CD_{AB} \frac{dx_A}{dz}$$

$$N_A \int_L^0 dz = -CD_{AB} \int_{x_{A1}}^{x_{A2}} \frac{1}{1 + 3x_A} dx_A$$

$$N_A(-L) = -CD_{AB} \int_{x_{A1}}^{x_{A2}} \frac{1}{1 + 3x_A} dx_A$$

$$\text{let } u = 1 + 3x_A$$

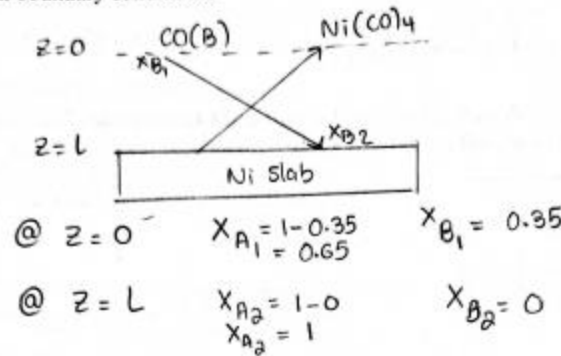
$$du = 3 dx_A$$

$$\frac{1}{3} du = dx_A$$

$$N_A = \frac{CD_{AB}}{3L} \ln \left(\frac{1 + 3x_{A2}}{1 + 3x_{A1}} \right)$$

$$N_A = \frac{PD_{AB}}{3RTL} \ln \left(\frac{1 + 3x_{A2}}{1 + 3x_{A1}} \right)$$

- b. Draw a schematic diagram of the concentration profile for the given system and specify your boundary conditions. (10 Points)



Ability to Formulate Engineering Problem

- c. Develop the final integrated equation for the flux of species B; be sure to use your boundary conditions. (15 Points)

$$\begin{aligned}
 4B &\rightarrow A \\
 N_A &= -\frac{N_B}{4} \\
 N_B &= -CD_{AB} \frac{dx_B}{dz} + x_B(N_A + N_B) \\
 &= -CD_{AB} \frac{dx_B}{dz} + x_B\left(-\frac{N_B}{4} + N_B\right) \\
 N_B &= -CD_{AB} \frac{dx_B}{dz} + \frac{3x_B N_B}{4} \\
 N_B - \frac{3x_B N_B}{4} &= -CD_{AB} \frac{dx_B}{dz} \\
 N_B \left(1 - \frac{3x_B}{4}\right) &= -CD_{AB} \frac{dx_B}{dz} \\
 N_B \int_0^L dz &= -CD_{AB} \int_{x_{B1}}^{x_{B2}} \frac{1}{1 - \frac{3x_B}{4}} dx_B \\
 (L) &= -CD_{AB} \int_{x_{B1}}^{x_{B2}} \frac{1}{1 - \frac{3x_B}{4}} dx_B
 \end{aligned}$$

$$\begin{aligned}
 \text{let } u &= 1 - \frac{3x_B}{4} \\
 du &= -\frac{3}{4} dx_B \\
 -\frac{4}{3} du &= dx_B \\
 N_B &= \frac{4CD_{AB}}{3L} \ln\left(\frac{4 - 3x_{B2}}{4 - 3x_{B1}}\right) \\
 &= \frac{4PD_{AB}}{3RTL} \ln\left(\frac{4 - 3x_{B2}}{4 - 3x_{B1}}\right) \\
 &= \frac{4PD_{AB}}{3RTL} \ln\left(\frac{4 - 3(0)}{4 - 3(0.35)}\right) \\
 N_B &= \frac{4PD_{AB}}{3RTL} (0.30)
 \end{aligned}$$

- d. Estimate the rate of production of nickel carbonyl (A), in mole/s-cm² of solid surface at steady state. The composition of the bulk gas phase ($z = 0$) is 35 mol% CO. The binary diffusivity is $D_{AB} = 20.0 \text{ mm}^2/\text{s}$. (10 Points)

$$\text{given } D_{AB} = 20 \text{ mm}^2/\text{s} \left(\frac{1 \text{ m}^2}{(10)^6 \text{ mm}^2} \right) = 0.2 \text{ cm}^2/\text{s}$$

$$P = 1 \text{ atm}$$

$$T = 350^\circ \text{K}$$

$$L = 0.7 \text{ mm} = 0.07$$

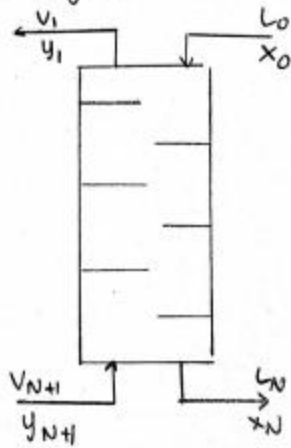
$$N_A = \frac{PD_{AB}}{3RTL} \ln \left(\frac{1 + 3X_{A2}}{1 + 3X_{A1}} \right)$$

$$= \frac{(1)(0.2)}{3(82.06)(350)(0.07)} \ln \left(\frac{1 + 3(1)}{1 + 3(0.65)} \right)$$

$$N_A = 1.01 \times 10^{-5} \text{ g.mol/cm}^2 \cdot \text{s}$$

Vivian Patthammavong

① Draw diagram



$$Y^* = 0.57x$$

$$V_{N+1} = 180 \text{ kmol/h}$$

$$y_{n+1} = 0.03$$

$$T = 30^\circ\text{C}, P = 110 \text{ kPa}$$

98% absorbed

$$\frac{L}{V} = 1.5 \left(\frac{L}{V} \right)_{\min}$$

$$\left(\frac{L}{V} \right)_{\min} = \frac{y_{n+1} - y_1}{x'_n - x_0}$$

$$\left(\frac{L}{V} \right)_{\min} = \frac{0.03 - 0.00062}{0.052 - 0}$$

$$\left(\frac{L}{V} \right)_{\min} = 0.565$$

$$x'_n = \frac{y_{n+1}}{0.57}$$

$$x'_n = \frac{0.03}{0.57}$$

$$x'_n = 0.052$$

$$\# \left(\frac{L}{V} \right)_{\text{actual}} = 1.5 \left(\frac{L}{V} \right)_{\min}$$

$$= 1.5(0.565)$$

$$\left(\frac{L}{V} \right)_{\text{actual}} = 0.848$$

$$\# x_N = ?$$

$$\left(\frac{L}{V} \right)_{\text{actual}} = \frac{y_{n+1} - y_1}{x_N - x_0}$$

$$x_N = \frac{y_{n+1} - y_1}{\left(\frac{L}{V} \right)_{\text{actual}}} = \frac{0.03 - 0.00062}{0.848}$$

$$x_N = 0.035 //$$

$$\# L_N = ?$$

$$L_N x_N + V_1 y_1 = V_{N+1} y_{N+1}$$

$$L_N = \frac{V_{N+1} y_{N+1} - V_1 y_1}{x_N} = \frac{(180)(0.03) - (174.71)(0.00062)}{0.035}$$

$$L_N = 151.19 \text{ kmol/h}$$

$$L_0 = ?$$

amount of ethyl alcohol leaving in $L_N(98.1\%) = (0.98)(5.4) = 5.292 \text{ kmol/h}$

$$L_0 = 151.19 \text{ kmol} - 5.292 \text{ kmol/h}$$

$$L_0 = \underline{145.89 \text{ kmol/h}} //$$

AVERAGE

Average Student Original Graded Assignment

10

Separation Process CHEG 3305 P02 (Spring 2022)

Exam 1 Time: ~~2 Hrs~~ Date: March 7 2022

1.5
Total points: 100

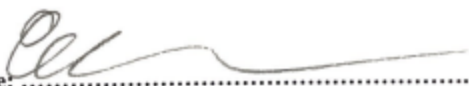
STUDENT NAME: Erron Williams DATE: 3/7/22

**Closed Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO RESTROOM
BREAKS NO COLLABORATION**

PROVIDE UNITS ON ALL CALCULATIONS AND ANSWERS

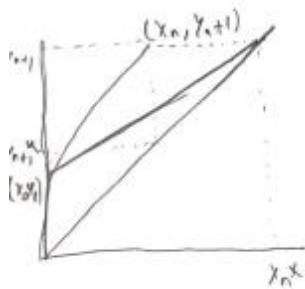
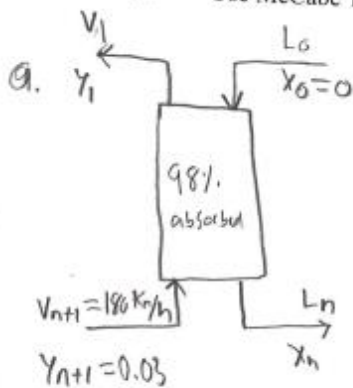
ANY DISHONESTY DURING THE EXAM WILL RESULT IN "F" GRADE

WORK ALL PROBLEMS ON THE QUESTION SHEETS AND DO NOT USE ANY SHEET
OF YOUR OWN

Student Signature: 

Problem 1 (40 Points) Molasses is fermented to produce a liquor containing ethyl alcohol. The CO_2 rich vapor containing a small amount of ethyl alcohol enters the column at 180 kmol/h at 30°C and 110 kPa , which contains $97\% \text{ CO}_2$ and $3\% \text{ ethyl alcohol}$. The alcohol can be recovered by absorption with pure water in a sieve tray tower. During the absorption process $98\% \text{ ethyl alcohol}$ is absorbed. The liquid flow rate (actual solute free absorbent) is 50% above the minimum liquid rate. The equilibrium relationship is $Y^* = 0.57 X$.

- Draw a schematic diagram of the absorption column and label it clearly showing all given information and unknown. (5 Points)
- Clearly Write the assumptions of McCabe-Thiele Method (5 Points)
- Determine the mole fraction of ethyl alcohol at the top of the column (7 Points)
- Calculate the pure water flow rate used to absorb ethyl alcohol. (8 Points)
- Determine the mole fraction of ethyl alcohol in water at the bottom of column (5 Points)
- Use McCabe Thiele Method to graphically calculate the theoretical number of stages (10 Points)



b. $I_n = \text{out}$

Isothermal and Isobaric? -2

$1 - 98 = 0.02 \text{ left}$

c. $(V_1)(Y_1) = 0.02 (V_{n+1})(Y_{n+1}) = 0.02 (180,000)(0.03)$

$(V_1)(Y_1) = 108 \text{ moles}$ assume $V_1 \approx V_{n+1}$

$Y_1 = \frac{108}{180,000} \rightarrow Y_1 = 6.0 \times 10^{-4}$

d. $V_{n+1} Y_{n+1} + L_0 X_0 = V_1 Y_1 + L_n X_n$ 0.0006

$Y_{n+1} = 0.57 X_n^* \rightarrow X_n^* = \frac{0.03}{0.57} = 0.053$

$(L/V)_{\min} = \frac{Y_{n+1} - Y_1}{X_n^* - X_0} = \frac{0.03 - (6.0 \times 10^{-4})}{0.053 - 0} = 0.555$

operating = $1.5 (L/V) = 1.5 (0.555) = 0.83$

$Y_{n+1} = 0.83 X_n + Y_1 \rightarrow \frac{Y_{n+1} - Y_1}{0.83} = X_n = \frac{0.03 - (6 \times 10^{-4})}{0.83}$

$$x_n = 0.035$$

$$V_{n+1} y_{n+1} + L_0 x_0 = V_1 y_1 + L_n x_n$$

$$L_n = \frac{(V_{n+1} y_{n+1}) - V_1 y_1}{x_n}$$

$$L_n = 151,200$$

$$L_0 = L_n (1 - x_n) = 151,200 (1 - 0.035)$$

$$L_0 = 145,908 \text{ moles H}_2\text{O fed}$$

Problem 2 (20 Points 2 Points each)

- a) For the determination of driving force in any mass transfer operation, the solubility of a species in a solvent, i.e., equilibrium distribution between phases is important. With the increase in temperature, solubility of a gas in liquid increases. Hence, absorption is done at higher temperature. On the contrary, desorption is done at lower temperature. (True/False) **False**
- b) Diffusivity in gas is proportional to $1/\mu$ (True/False) **True**
- c) Which of the following is NOT true of diffusion in gases, liquids and solids?
- The rate of diffusion depends on the component diffusing; the medium is not very important
 - The rates of diffusion in liquids and gases is different by several orders of magnitude
 - The rates of diffusion in liquids and solids is different by several orders of magnitude
 - The rate of diffusion in solids and the rate of diffusion in liquids are both slower than in gases
- d) Mass transfer is driven by concentration gradient as well as by pressure gradient and electrical gradient. (True/False) **False**

Answer the following two questions using the plot below (2points each)

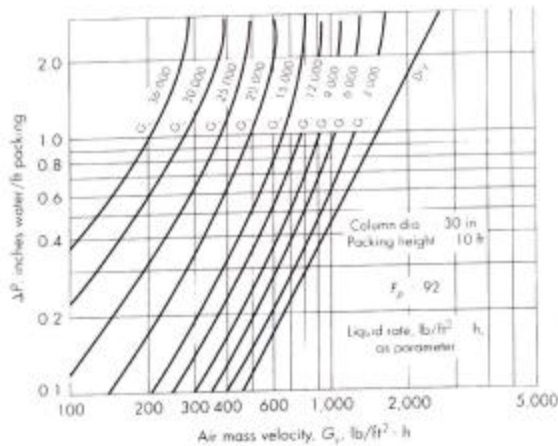


FIGURE 18.4
Pressure drop in a packed tower for air-water system with 1-in. Intalox saddles. (1,000 lb/ft²·h = 1,356 kg/m²·s; 1 in. H₂O/m = 817 Pa/m)

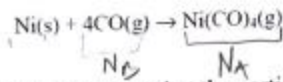
- e. At very low liquid rates, the effective cross section of the packing is not appreciably different from that of dry packing and pressure drop is due to flow through a series of variable openings in the bed that is called channeling. (True / False) 2
- f. From the above figure write down what is the pressure drop when flooding takes place..... (fill in the blank) 1, 0 in water / ft 2
- g. Factors that may lead to flooding:
- High inlet gas flow rates
 - Low liquid circulation rates
 - Small diameter towers
 - d All of the above
- h. The process of the purification of natural gas by contact with an ethanolamine (alkaline) solution is called absorption (True / False)
- i. Write only the general equation for diffusion of gases A and B

$$N_A = - \frac{D_{AB}}{R_T (Z_2 - Z_1)} + (N_A + N_B) X$$

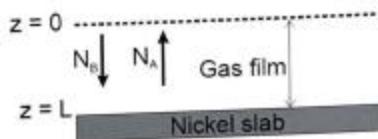
-2

$$-\frac{P_{A0}}{RT} \frac{dP}{dz} = -(N_A + N_B) \quad \frac{D_{AB} P}{RT(z-z_1)P_{A0}} \quad N_A = \frac{D_{AB}}{L} \frac{dX}{dz} + X(N_A + N_B)$$

Problem 3 (a-d) (40 points) Nickel carbonyl (A) is produced by passing carbon monoxide (B) at 350 K and 1 atm over a nickel slab. The following reaction takes place at the solid surface:



The reaction is very rapid, so that the partial pressure of CO at the metal surface is essentially zero. The gases diffuse through a film with a thickness $L = 0.7$ mm.



Ability to Identify Engineering Problem

- a. List all the assumptions; simplify the general mass transfer equation for species A.

(5 Points)

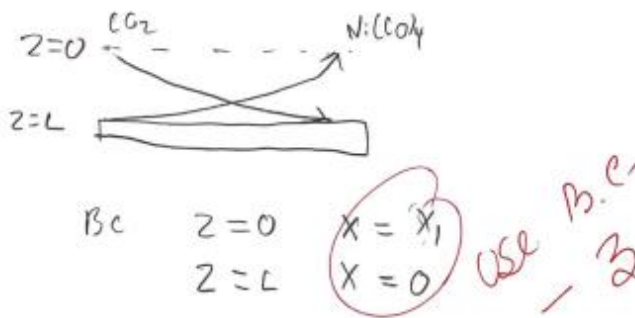
$$\frac{N_A}{1} = \frac{-N_B}{4} \quad \text{isobaric, isothermal} \quad -2$$

$\rightarrow N_B = 4N_A$

$$N_A = \frac{-C_A D_{AB}}{C_T} \frac{dX}{dz} + X(N_A + N_B)$$

$$N_A = -D_{AB} \frac{C_A}{C_T} \frac{dX}{dz} + X(N_A - 4N_A)$$

- b. Draw a schematic diagram of the concentration profile for the given system and specify your boundary conditions. (10 Points)



Ability of Formulate Engineering Problem

- c. Develop the final integrated equation for the flux of species B; be sure to use your boundary conditions. (15 Points)

$$N_A = -D_{AB} \frac{c_A}{c_T} \frac{dx}{dz} + x(N_A - 4N_A)$$

$$N_A(1-3x) = -\frac{D_{AB}c_A}{c_T} \frac{dx}{dz}$$

$$N_A \int_L^0 dz = -\frac{D_{AB}c_A}{c_T} \int_0^{x_1} \frac{dx}{(1-3x)}$$

$$N_A(-L) = -\frac{D_{AB}c_A}{c_T} \ln \left(\frac{1}{1-3x_1} \right)$$

$$\ln(1-3x_1) = \ln(1-30)$$

$$N_B = ?$$

Ability of solve Engineering Problem

- d. Estimate the rate of production of nickel carbonyl (A), in mole/s·cm² of solid surface at steady state. The composition of the bulk gas phase ($z = 0$) is 35 mol% CO. The binary diffusivity is $D_{AB} = 20.0 \text{ mm}^2/\text{s}$. **(10 Points)**

$$N_A = \frac{D_{AB} C_A}{C_T L} \ln \frac{1}{(1-3x)}$$
$$= \frac{(20.0 \text{ mm}^2/\text{s}) (C_A)}{(C_T) (0.7 \text{ m})} \ln \frac{1}{(1-3(0.35))}$$

~~0.0~~
-7

BELOW AVERAGE

Below Average Student Original Graded Assignment

44
Separation Process CHEG 3305 P02 (Spring 2022)

Exam I Time: ~~2 Hrs~~ Date: March 7 2022

1.5 Hrs

Total points: 100

STUDENT NAME: Isaiah Waters DATE: 3/7/2022

Closed Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO RESTROOM
BREAKS NO COLLABORATION

PROVIDE UNITS ON ALL CALCULATIONS AND ANSWERS

ANY DISHONESTY DURING THE EXAM WILL RESULT IN "F" GRADE

WORK ALL PROBLEMS ON THE QUESTION SHEETS AND DO NOT USE ANY SHEET
OF YOUR OWN

Student Signature: Isaiah Waters

Problem 1 (40 Points) Molasses is fermented to produce a liquor containing ethyl alcohol. The CO_2 rich vapor containing a small amount of ethyl alcohol enters the column at 180 kmol/h at 30°C and 110 kPa , which contains $97\% \text{ CO}_2$ and $3\% \text{ ethyl alcohol}$. The alcohol can be recovered by absorption with pure water in a sieve tray tower. During the absorption process 98% ethyl alcohol is absorbed. The liquid flow rate (actual solute free absorbent) is 50% above the minimum liquid rate. The equilibrium relationship is $Y^* = 0.57 X$.

- Draw a schematic diagram of the absorption column and label it clearly showing all given information and unknown. (5 Points)
- Clearly Write the assumptions of McCabe-Thiele Method (5 Points)
- Determine the mole fraction of ethyl alcohol at the top of the column (7 Points)
- Calculate the pure water flow rate used to absorb ethyl alcohol. (8 Points)
- Determine the mole fraction of ethyl alcohol in water at the bottom of column (5 Points)
- Use McCabe Thiele Method to graphically calculate the theoretical number of stages (10 Points)

b) assumptions of McCabe-Thiele Method: operating & equilibrium curves are both linear

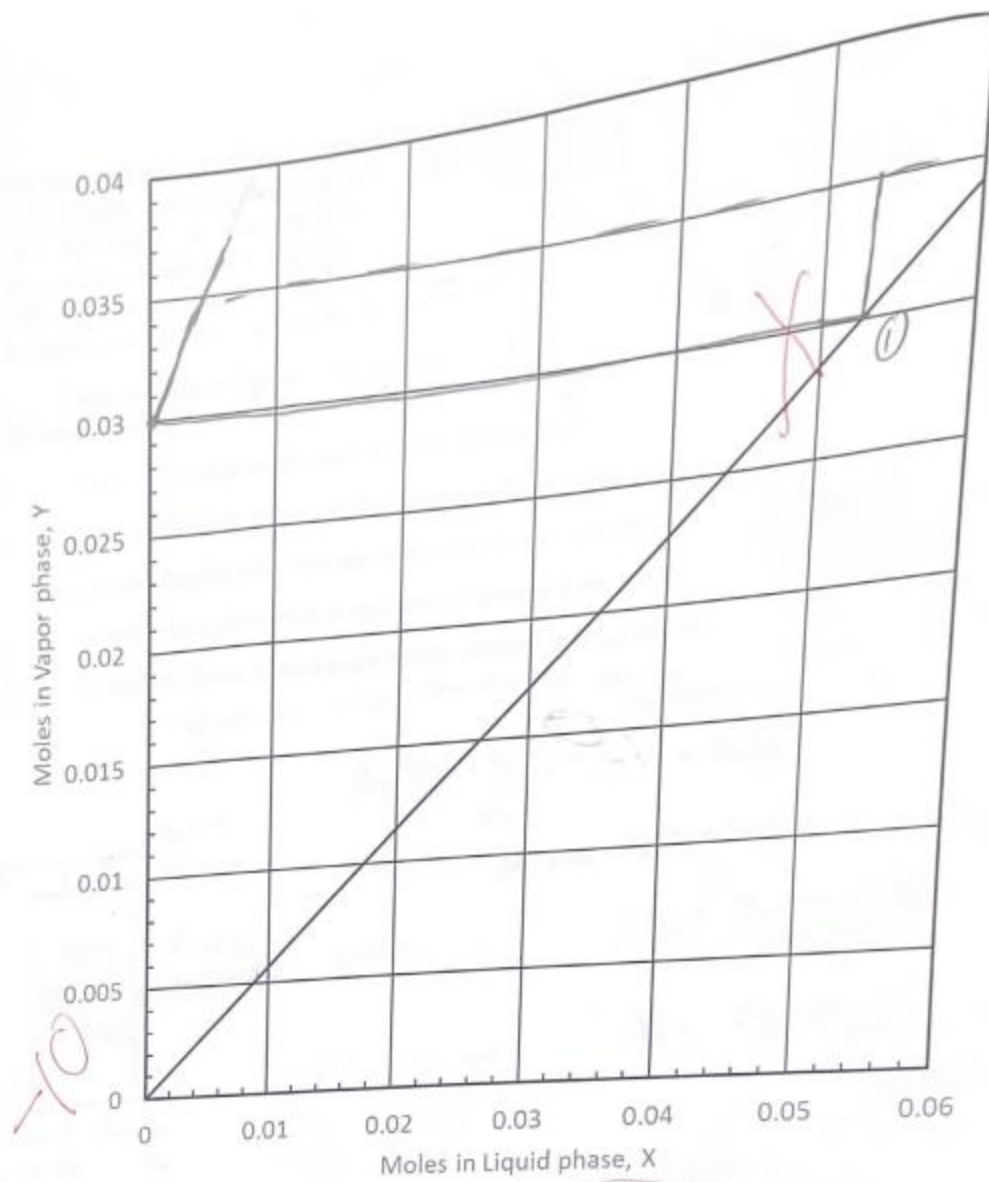
a)

$x_0 = 0$
 L_0
 $T = 30^\circ\text{C}$
 $P = 110 \text{ kPa}$
 $p_A = H x_A$
 $98\% \text{ ethyl alcohol absorbed}$
 $y_{n+1} = 0.03$
 $V_{n+1} = 180 \text{ kmol/h}$
 x_n
 L_n

$y_{n+1} V_{n+1} + x_0 L_0 = y_1 V_1 + x_n L_n$
 $y_{n+1} V_{n+1} = y_1 V_1 + x_n L_n$
 $x_n = \frac{y_{n+1} V_{n+1} - y_1 V_1}{L_n}$
 $x_n = \frac{5.4 \text{ kmol/h} - 0.108 \text{ kmol/h}}{L_n}$
 $L_n = 1.5 \left(\frac{1}{2}\right) \text{ min.}$
 $V_1 + L_n = L_0 + V_{n+1}$
 $L_n - L_0 = V_{n+1} - V_1$
 $L_n - 1.5(180) = 5.292$
 $L_n = 275.292 \text{ kmol/h}$
 $x_n = \frac{5.4 - 0.108}{275.292}$
 $x_n = 0.019$

ethyl alcohol entering vapor
 $y_{n+1} V_{n+1} = (0.03)(180)$
 $= 5.4 \text{ kmol/h}$
 ethyl alcohol absorbed
 $0.98(5.4 \text{ kmol/h})$
 $= 5.292 \text{ kmol/h}$
 $x_n L_n$
 Total exiting vapor
 $V_1 = 0.02(5.4) + 174.6$
 $V_1 = 174.708 \text{ kmol/h}$
 $y_1 V_1 = 0.02(174.708)$
 $= 3.494 \text{ kmol/h}$
 $y_1 = 0.02$

$\text{CO}_2 \text{ entering/exiting}$
 $(180 \text{ kmol/h})(0.97) = 174.6 \text{ kmol/h}$
 ethyl alcohol exiting as vapor
 $0.02 y_{n+1} V_{n+1} = 0.02(0.03)(180)$
 $y_1 V_1 = 0.108 \text{ kmol/h}$



Slope: $\frac{y_n - y_1}{x_n - x_0} = \frac{0.03 - (6 \times 10^{-4})}{0.019} = 1.547$

$y = 1.547x + 0.03$ $\leftarrow y_{n+1}$

4

2 theoretical stage required

Problem 2 (20 Points 2 Points each)

- a) For the determination of driving force in any mass transfer operation, the solubility of a species in a solvent, i.e., equilibrium distribution between phases is important. With the increase in temperature, solubility of a gas in liquid increases. Hence, absorption is done at higher temperature. On the contrary, desorption is done at ~~lower~~ ^{higher} temperature. (True/False) ~~True~~ ^{False}
- b) Diffusivity in gas is proportional to $1/\mu$ (True/False) ~~True~~ ^{False; $\frac{1}{P}$}
- c) Which of the following is NOT true of diffusion in gases, liquids and solids?

- a. The rate of diffusion depends on the component diffusing; the medium is not very important
- b. The rates of diffusion in liquids and gases is different by several orders of magnitude
- c. The rates of diffusion in liquids and solids is different by several orders of magnitude
- d. The rate of diffusion in solids and the rate of diffusion in liquids are both slower than in gases
- d) Mass transfer is driven by concentration gradient as well as by pressure gradient and electrical gradient. (True/False) ~~True~~ ^{False}

Answer the following two questions using the plot below (2points each)

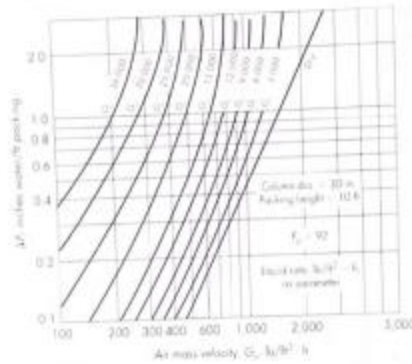


FIGURE B4
Pressure drop in a packed tower for air-water system with 1-in. Intalox saddles. (1,000 ft) = 1.356 kPa/m; 1 in. H₂O = 0.491 Pa/m

mass velocity

$$1 \text{ ft} = 12 \text{ in}$$

$$(30 \text{ in}) \left(\frac{1 \text{ ft}}{12 \text{ in}} \right) = 2.5 \text{ ft}$$

Vol of column

$$\frac{\pi}{2} d^2 h = \frac{\pi}{2} (2.5 \text{ ft})^2 (10 \text{ ft})$$

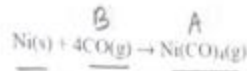
$$= 39.27 \text{ ft}^3$$

$$(3.927 \text{ ft}^3)$$

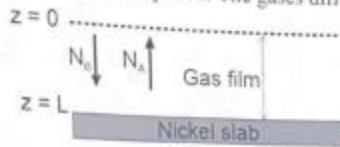
- e. At very low liquid rates, the effective cross section of the packing is not appreciably different from that of dry packing and pressure drop is due to flow through a series of variable openings in the bed that is called channeling. (True/ False)
- f. From the above figure write down what is the pressure drop when flooding takes place..... (fill in the blank) ✓
- g. Factors that may lead to flooding:
- High inlet gas flow rates
 - Low liquid circulation rates
 - Small diameter towers
 - All of the above ✓
- h. The process of the ^{stripping?} purification of natural gas by contact with an ethanolamine (alkaline) solution is called absorption (True/ False) ✓
- i. Write only the general equation for diffusion of gases A and B

$$N_A = -D_{AB} \frac{dc_A}{dz} + \frac{N_A + N_B}{\gamma} \quad \checkmark$$

Problem 3 (a-d) (40 points) Nickel carbonyl (A) is produced by passing carbon monoxide (B) at 350 K and 1 atm over a nickel slab. The following reaction takes place at the solid surface:



The reaction is very rapid, so that the partial pressure of CO at the metal surface is essentially zero. The gases diffuse through a film with a thickness $L = 0.7$ mm.



Ability to Identify Engineering Problem

- a. List all the assumptions; simplify the general mass transfer equation for species A.

(5 Points)

Steady-state ?
Assume $C_T = 1$

assumptions

$$N_A = -D_{AB} \frac{dc_A}{dz} + \frac{(N_A + N_B)}{C_T}$$

$$-r_B = 4r_A$$

$$N_B = -4N_A$$

$$N_A = -D_{AB} \frac{dc_A}{dz} + \frac{(N_A - 4N_A)}{C_T}$$

$$N_A = -D_{AB} \frac{dc_A}{dz} - \frac{3N_A}{C_T}$$

$$N_A + \frac{3N_A}{C_T} = -D_{AB} \frac{dc_A}{dz}$$

$$C_T = 1$$

$$4N_A = -D_{AB} \frac{dc_A}{dz}$$

$$\int_{z_1}^{z_2} 4N_A dz = \int_{c_{A1}}^{c_{A2}} -D_{AB} dc_A$$

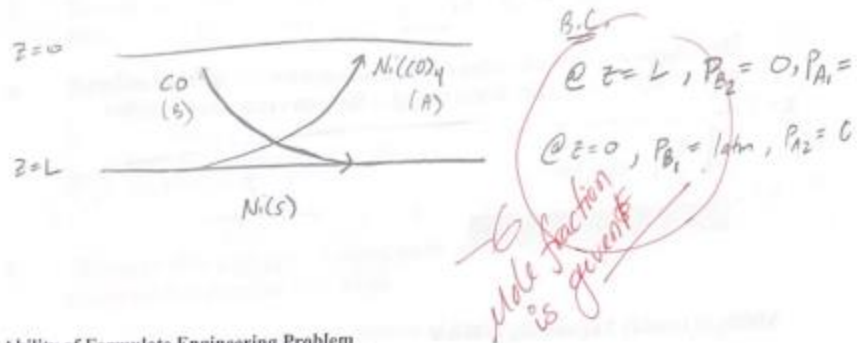
$$4N_A(z_2 - z_1) = -D_{AB}(c_{A1} - c_{A2})$$

not here

In terms of partial pressure

$$N_A = \frac{-D_{AB}(P_{A1} - P_{A2})}{4RT(z_2 - z_1)}$$

- b. Draw a schematic diagram of the concentration profile for the given system and specify your boundary conditions. (10 Points)



Ability of Formulate Engineering Problem

- c. Develop the final integrated equation for the flux of species B; be sure to use your boundary conditions. (15 Points)

$$N_B = \frac{D_{AB}}{RT(z_2 - z_1) P_{B,LM}} (P_{A1} - P_{A2})$$

$$\int_{z=0}^{z=L} 4N_A dz = \int_{P_A=P_{A1}}^{P_A=P_{A2}} \frac{-D_{AB}}{RT} dP_A$$

$$N_A = \frac{D_{AB} (P_{A1} - P_{A2})}{RT L}$$

Ability of solve Engineering Problem

- d. Estimate the rate of production of nickel carbonyl (A), in mole/s-cm² of solid surface at steady state. The composition of the bulk gas phase ($z = 0$) is 35 mol% CO. The binary diffusivity is $D_{AB} = 20.0 \text{ mm}^2/\text{s}$. (10 Points)

$$N_A = \frac{D_{AB} (P_A - P_{A2})}{RTL} \quad \text{how did you get this} \quad -10$$

$$= \frac{(20.0 \text{ mm}^2/\text{s}) \left(\frac{10^{-3} \text{ m}}{\text{mm}}\right)^2 (1 \text{ atm} - 0 \text{ atm})}{(0.0821 \text{ atm} \cdot \text{m}^3 \cdot \text{K}^{-1} \cdot \text{mol}^{-1}) (350 \text{ K}) (0.7 \text{ mm}) \left(\frac{10^{-3} \text{ m}}{\text{mm}}\right)}$$

$$N_A = 994 \text{ mol/m}^2 \cdot \text{s}$$

Separation Processes Spring 2022

Quiz 1

TOPICS COVERED IN Quiz 1

- 1. Principles of Mass Transfer**
- 2. Calculating molar flux of evaporating water**

**CHEG 3305 P02 Separation Processes
Spring 2022**

**Quiz #1 QUESTIONS, SOLUTION,
AND GRADING SCHEME**

Separation Processes

CHEG 3305

Quiz 1 Date: January 31 2022

Water evaporating from a pond does so as if it were diffusing across an air film 0.50 cm thick. Air is not diffusing in water. The diffusion coefficient of water in 20°C air is about 0.25 cm²/s. If the atmospheric air is 50% saturated, answer the following questions:

1. Draw a schematic diagram of the mass transfer process.
2 Points
2. Calculate the molar flux of evaporating water across the air film.
5 Points
3. How fast will the water level drop in a day?
3 Points

Given vapor pressure of water at 20°C is 17.54 mm.

ABOVE AVERAGE

Above Average Student Original Graded Assignment

Separation Process: Quiz 1

Date: January 31, 2022

1. Water evaporating from a pond does so as if it were diffusing across an air film 0.50 cm thick. The diffusion coefficient of water in 20°C air is about 0.25 cm²/s. If the atmospheric air is 50% saturated, answer the following questions:

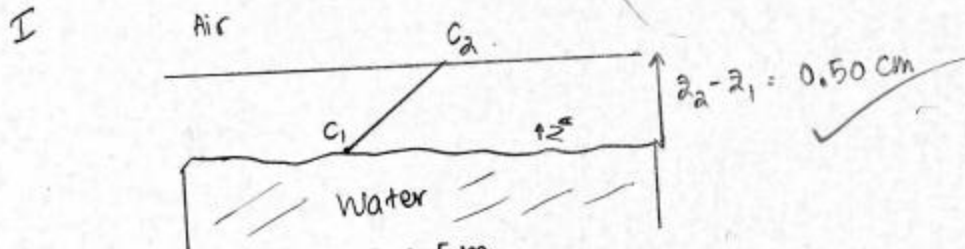
- Draw a schematic diagram of the mass transfer process. 2 Points
 - Calculate the molar flux of evaporating water across the air film. Consider equimolar diffusion. 5 Points
 - How fast will the water level drop in a day? 3 Points
- Given vapor pressure of water at 20°C is 17.54 mm. Hg

$$N_A = -D_{AB} \frac{dC_A}{dz} + \frac{C_A}{C_T} (N_A + N_B)$$

Total Concentration

$$N_A = -\frac{D_{AB}}{RT} \frac{dp_A}{dz} + \frac{p_A}{P} (N_A + N_B)$$

Total Pressure



II

$$z_2 - z_1 = 0.50 \text{ cm} = 0.005 \text{ m}$$

$$P_A = 0.5 P_{\text{sat}}$$

$$T = 20^\circ\text{C} + 273 = 293 \text{ K}$$

$$P_{\text{sat}} = 17.54 \text{ mmHg} \times \frac{1 \text{ atm}}{760 \text{ mmHg}} = 0.0231 \text{ atm}$$

$$D_{AB} = 0.25 \text{ cm}^2/\text{s} \times \frac{1 \text{ m}^2}{(100 \text{ cm})^2} = 2.5 \times 10^{-5} \text{ m}^2/\text{s}$$

$$N_A = ?$$

$$N_A = -\frac{D_{AB}}{RT} \frac{dP_A}{dz} + \frac{P_A}{P} (N_A + N_B)$$

Equimolar diffusion $N_A = -N_B$

$$N_A = \frac{-D_{AB}(P_A - P_{sat})}{RT(z_2 - z_1)} = \frac{D_{AB}(P_{sat} - P_A)}{RT(z_2 - z_1)} = \frac{D_{AB}(P_{sat} - 0.5P_{sat})}{RT(z_2 - z_1)}$$

$$= \frac{(2.5 \times 10^{-5})(0.5P_{sat})}{RT(z_2 - z_1)}$$

$$= \frac{(2.5 \times 10^{-5})(0.5)(0.0231)}{(0.0821)(293)(0.005)} \checkmark$$

$$N_A = \boxed{2.4 \times 10^{-6} \text{ kg.mol/m}^2.\text{s}}$$

III How fast the water drop in a day?

$$2.4 \times 10^{-6} \frac{\text{kg.mol}}{\text{m}^2.\text{s}} \times \frac{3600\text{s}}{1\text{h}} \times \frac{24\text{h}}{1\text{day}} \times \frac{1\text{m}}{1000\text{kg}} \times \frac{18\text{kg}}{1\text{kg.mol}}$$

$$\text{rate of water} = \boxed{3.73 \times 10^{-3} \text{ m/day}} \checkmark$$

AVERAGE

Average Student Original Graded Assignment

Name: Ohwatumini V. Alade

CHEG 3305

6

Separation Process: Quiz 1

Date: January 31, 2022

1. Water evaporating from a pond does so as if it were diffusing across an air film 0.50 cm thick. The diffusion coefficient of water in 20°C air is about 0.25 cm²/s. If the atmospheric air is 50% saturated, answer the following questions:

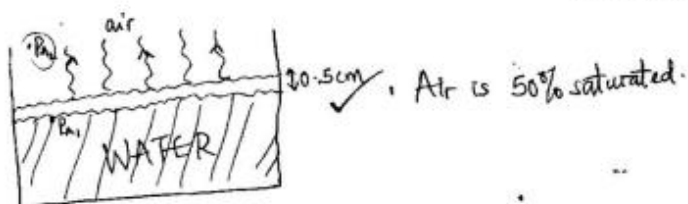
- I. Draw a schematic diagram of the mass transfer process. 2 Points
 - II. Calculate the molar flux of evaporating water across the air film. Consider equimolar diffusion. 5 Points
 - III. How fast will the water level drop in a day? 3 Points
- Given vapor pressure of water at 20°C is 17.54 mmHg

$$N_A = -D_{AB} \frac{dC_A}{dz} + \frac{C_A}{C_T} (N_A + N_B)$$

Total Concentration

$$N_A = -\frac{D_{AB}}{RT} \frac{dp_A}{dz} + \frac{p_A}{P} (N_A + N_B)$$

Total Pressure



Assumptions:
- Equimolar diffusion
- Const. Pressure & temp.

$$D_{AB} = 0.25 \text{ cm}^2/\text{s}$$

$$T = 20^\circ\text{C} = 293\text{K}$$

$$J_A = ?$$

$$J_A = -\frac{D_A dP}{RT dz}$$

$$P_{A1} = 17.54 \text{ mmHg} = \left(\frac{17.54}{760} \times 101325 \right) = 2338.47 \text{ Pa}$$

$$P_{A2} = 50\% \text{ saturated.}$$

$$P_{A2} = 0$$

$$J_A dz = \frac{-D_{AB} dP}{RT} \quad \text{from } J_A dz = -D_{AB} dC_A$$

where $C_A = \frac{P}{RT}$

Integrating both side

$$J_A \int dz = \frac{-D_A}{RT} \int dP$$

$$J_A (0.5-0) = \frac{-0.25}{8314 \times 293} (0 - 2338.74)$$

$$J_A = \frac{-0.25 \cdot (0 - 2338.74)}{8314 \times 293 \times 0.5} \quad -2$$

$$J_A = 0.00048 \approx 4.8 \times 10^{-4} \text{ kg/cm}^2\text{s}$$

(ii) $t = ?$ for water level to drop in a day.

$$1 \text{ day} = 24 \text{ hrs.} = 86400 \text{ sec}$$

In one second, 0.00048 kg/cm^2 diffuses

In 86400 seconds, $x \text{ kg/cm}^2$ diffuses

$$\text{So, } x = 86400 \times 0.00048$$

$$x = 41.472 \text{ kg/cm}^2\text{s} \quad -2$$

BELOW AVERAGE

Below Average Student Original Graded Assignment

Separation Process: Quiz 1

Date: January 31, 2022

1. Water evaporating from a pond does so as if it were diffusing across an air film 0.50 cm thick. The diffusion coefficient of water in 20°C air is about 0.25 cm²/s. If the atmospheric air is 50% saturated, answer the following questions:

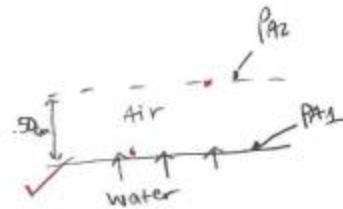
- Draw a schematic diagram of the mass transfer process. 2 Points
 - Calculate the molar flux of evaporating water across the air film. Consider equimolar diffusion. 5 Points
 - How fast will the water level drop in a day? 3 Points
- Given vapor pressure of water at 20°C is 17.54 mmHg

$$N_A = -D_{AB} \frac{dC_A}{dz} + \frac{C_A}{C_T} (N_A + N_B)$$

Total Concentration

$$N_A = -\frac{D_{AB}}{RT} \frac{dp_A}{dz} + \frac{p_A}{P} (N_A + N_B)$$

Total Pressure



given:

(water) $D_{AB} @ 20^\circ\text{C} = 0.25 \text{ cm}^2/\text{s} = 2.5 \times 10^{-5} \text{ m}^2/\text{s}$

Vapor pressure water @ 20°C = 17.54 mmHg

$= \frac{17.54 \text{ mmHg}}{760 \text{ mmHg}} = 0.023078947 \text{ atm}$

Air = 50% saturated

$T = 20^\circ\text{C} + 273 = 293 \text{ K}$

Thickness = $\frac{0.50 \text{ cm}}{1} \cdot \frac{3 \text{ m}}{100 \text{ cm}} = 5.3 \times 10^{-3} \text{ m}$

$M_{H_2O} = 18.02 \text{ g/mol}$

1 day = 24 hr = 86400 seconds

We know:

$R = 82.06 \times 10^{-3} \text{ atm} \cdot \text{m}^3/\text{kmol} \cdot \text{K}$

1 atm = 760 mmHg

$\frac{0.25 \text{ cm}^2}{1} \cdot \frac{1 \text{ m}^2}{(100 \text{ cm})^2} = 2.5 \times 10^{-5} \text{ m}^2$

$N_A = -2.5 \times 10^{-5} \text{ m}^2 \left[\frac{0.023078947}{5.3 \times 10^{-3} \text{ m}} + \right]$

**CHEG 3305 P02 Separation Processes
Spring 2022**

Final Project

TOPICS COVERED IN Project 1

- 1. Use Aspen HYSYS to design Distillation column**

**CHEG 3305 P02 Separation Processes
Spring 2022**

**Final Project # QUESTIONS, SOLUTION,
AND GRADING SCHEME**

Final Project CHEG 3305

This is a group project. The project is **due on May 6 2022**

Project Goals

The goals of the project are

- (1) to give the students more experience with real world problems beyond the scope of those typically included in undergraduate textbooks,
- (2) to connect major concepts from the course, using material balance, energy balance and phase equilibrium equations
- (3) to provide students with opportunities to explore industrial applications in areas of interest. The activity connects course concepts to real world applications and requires students to design their own case studies through exploring the research and patent literature.

Problem Statement

Light naphtha is a mixture produced by distillation of crude oil. Light naphtha primarily contains alkane compounds (paraffin) and it can be blended into gasoline. The octane value of methyl substituted alkanes (iso paraffin) is higher than that of starting chain compounds (normal paraffin) so it's often advantageous to isomerize the light naphtha to increase the proportion of branched compounds.

A simple naphtha isomerization process has a feed of 10000 barrels per day of a 50 wt% mixture of n-hexane and methyl pentane. The feed is heated and sent to a reactor where it is brought to equilibrium at 1300KPa and 250°C. The reactor products are cooled to the dew point and fed to a distillation column operated at 300KPa. The bottom product of the distillation is rich in n-hexane and is recycled to the reactor feed. An overall conversion of 95% is achieved. Simulate the process to determine the recycle flow rate and composition.

How to submit your report :

Final report :

The final report for the project should follow the following formatting. Point breakdowns for the 100 points allocated to the final report are indicated in parenthesis. Grammar and formatting errors may be deducted from any relevant sections. The report must be submitted electronically via ecourse. No handwritten notes are allowed, and all equations must be typed. Label all of the following sections and subsections in the order listed.

1. Title Page (1) – course number, project title, project group number, group members, date
 - a) Table of Contents(1)
 - b) List of tables (1)
 - c) List of figures (1)
 - d) Page number on each page (except title page) (1)
2. Executive Summary (10) – A 1/2-page, or less, statement that should contain the objective (1), results (2), and conclusions (3). The purpose is to succinctly convey why the project was done, what the objective was, what the result of the work was.

For Example: The objective of the study is to design a separation unit using Aspen for synthesis of Ethyl Benzene process which consists of reactors and distillation column.

3. Process Description. (25 points)

4. Process Simulation and results (40 Points)

- Present the numbers in a way that is clearly stated and identified . Mention the graphs or figures you have obtained from Aspen HYSYS.

Primary Control objectives such as reboiler heat input, reflux ratio

- Recycle stream properties
- Acceptable composition
- Is further processing required?

The graphs or figures you have obtained from Aspen HYSYS.

- Estimate the number of ideal stages required and feed stage

5. Recommendations for further development (10 points)

6. Conclusions. (5 points)

7. References (5 points)

Hints: To get an initial estimate of the distillation column conditions, first simulate using a shortcut column model. Consider methyl pentane as heavy key. Assume mole fraction of methyl pentane at the bottoms is 0.2. With recycle not closed the short column will give you minimum reflux.

- If a group member is absent for the work and does not help leave his/her name from the report. Attach a short note explaining why this member's name not included.
- All groups must attach their HYSYS project in canvas along with the report
- Do not attach the entire Aspen HYSYS results printout
- At the end of the project, you will be asked to complete a confidential report evaluating your group members.

ABOVE AVERAGE

Above Average Student Original Graded Assignment

Prairie View A&M
Roy G. Perry College of Engineering



Chemical Reaction Engineering

CHEG 3306- P02

Final Project

Submitted by:

Berenice Rincon

Edgar Mendoza

Meibryth Salas

Dynasty Stephenson

Submitted To: Dr. Nabila Shamim

Due Date: May 6, 2022

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Executive Summary

The objective of this project was to provide us with a real-world application of the concepts we have been learning about for distillation columns. The isomerization of Naphtha involved material balance, energy balance, and phase equilibrium techniques which allowed us to explore industrial applications. First, we needed to design our process using a short distillation column to give us a range of parameters to eventually design our full process design. Our first trial calculated that we needed 30 minimal trays, 62 actual trays, the optimal stage was at 40, an external reflux ratio of 8.9, a minimum reflux ratio of 7.5, a methyl pentane (light key) composition of .2, n-hexane (heavy key) composition of .8 in the liquid phase and .23 and .77 in the vapor phase respectively. Finally, using those parameters for our complete distillation process our results indicated that our distillation column required 50 trays and our optimal feed stage was at 33. From the 10,000 barrels/day we calculated a value of 459 kgmol/h molar flow rate, which Aspen Hysys confirmed by it calculating a value of 494.6 kgmol/h. Our recycle stream calculated a .93 mole fraction composition for n-hexane (heavy key) and .067 for methyl pentane (light key). In conclusion, for our isomerization process of light naphtha, we had to first use a short distillation column to extract a range of parameters to eventually be able to run a complete process which exposed us to real-world industrial applications.

Problem Statement

Light naphtha is a mixture produced by the distillation of crude oil. Light naphtha primarily contains alkane compounds (paraffin) and it can be blended into gasoline. The octane value of

methyl-substituted alkanes (isoparaffin) is higher than that of starting chain compounds (normal paraffin) so it's often advantageous to isomerize the light naphtha to increase the proportion of branched compounds. A simple naphtha isomerization process has a feed of 10,000 barrels per day of a 50 wt.% mixture of n-hexane and methyl pentane. The feed is heated and sent to a reactor where it is brought to equilibrium at 1300kPa and 250°C. The reactor products are cooled to the dew point and fed to a distillation column operated at 300kPa. The bottom product of the distillation is rich in n-hexane and is recycled into the reactor feed. An overall conversion of 95% is achieved. Simulate the process to determine the recycle flow rate and composition.

Process Description

Isomerization is the process of transforming straight-chained hydrocarbon components into branched hydrocarbon components with a higher-octane number. With Light naphtha, isomerization has been recognized in the refining industry for many years because of its ability to higher the octane number in gasoline. The isomerization process converts light naphtha into higher-value gasoline by changing the molecular shape and raising its octane content. This process of isomerization is a simple and cost-effective process for octane enhancement compared with other octane-improving processes available. The isomerization process is being used by many countries worldwide because it provides a way to improve the quality of fuels to decrease the impact of environmental and health issues. The high demand for clean fuels and premium gasoline grades makes the isomerization process common worldwide.

Light Naphtha is primarily composed of alkane compounds, also known as paraffin, and is mixed to create gasoline. To get an initial estimate of the distillation column conditions a simulation using a short column model was used as shown in figure 1. In the model, the feed for the distillation column unit was composed of 50 wt% of n-hexane and methyl pentane. The feed was fed into a mixer and sent to a heater where it was heated and sent to a Gibbs reactor where it was brought to equilibrium at 1300 KPa and 250°C. The reactor products were then cooled to the dew point and fed to a distillation column operated at 300 KPa. The mole fraction of the light key 2-methyl pentane at the bottoms was assumed to be 0.2. With the given conditions, and with the recycle not being closed, the shortcut model estimated a minimum reflux of 7.5 and an external

reflux ratio of 8.9 as shown in table 3. Using the shortcut model, we calculated that we need 30 minimum number of trays, 62 theoretical trays, and an optimal number of trays of 41, as shown in table 4. The parameters obtained from the shortcut model were used for our complete distillation column. The results from the complete distillation column with the inputs of the shortcut model indicated that our column required a flow rate of 494.6 kgmol/h

Process Simulation and Results

During this process simulation, we calculated the reboiler heat input and reflux ratio which is 61.9 degrees Celsius and 7.7 respectively found in Figure 3. The recycle stream includes a temperature of 107.8 degrees Celsius, a pressure of 1300kPa, and 218.7 kgmole/h which can be found in Figure 3. Yes, it is an acceptable composition because the light key and heavy key was identified, and the overall conversion was accurate. No, in our estimation the overall process is at 90 percent with the conditions we used in the project. Realist 90 percent efficient is a great efficiently for this distillation column and to try to increase the overall conversion would cost extra money, time, and people.

Stream Name	1	Vapour Phase	Liquid Phase
Vapour / Phase Fraction	0.0002	0.0002	0.9998
Temperature [C]	106.3	106.3	106.3
Pressure [kPa]	300.0	300.0	300.0
Molar Flow [kgmole/h]	3.820	8.367e-004	3.820
Mass Flow [kg/h]	329.2	7.210e-002	329.2
Std Ideal Liq Vol Flow [m3/h]	0.4978	1.090e-004	0.4977
Molar Enthalpy [kJ/kgmole]	-1.829e+005	-1.569e+005	-1.829e+005
Molar Entropy [kJ/kgmole-C]	88.63	151.7	88.62
Heat Flow [kJ/h]	-6.987e+005	-131.3	-6.986e+005
Liq Vol Flow @Std Cond [m3/h]	0.4954	1.085e-004	0.4953
Fluid Package	Basis-1		
Utility Type			

Table 1: Input Conditions for Shortcut Distillation Column

	Mole Fractions	Liquid Phase	Vapour Phase
2-Mpentane	0.2000	0.2000	0.2332
n-Hexane	0.8000	0.8000	0.7668

Table 2: Mole Composition of 2-Mpentane and n-Hexane for Shortcut Distillation Column

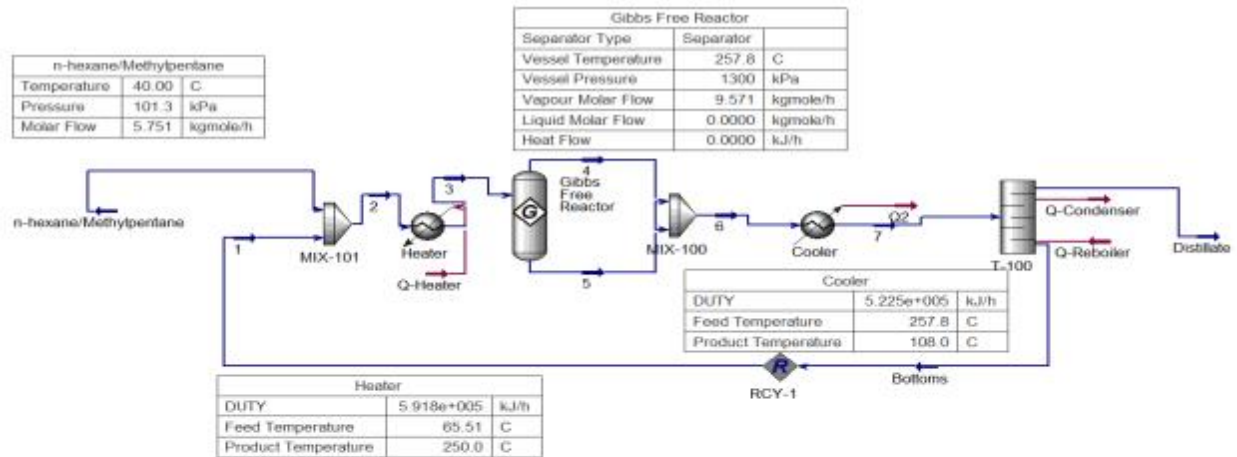


Figure 1: Schematic for Shortcut Distillation Column

Components		
	Component	Mole Fraction
Light Key in Bottoms	2-Mpentane	0.2000
Heavy Key in Distillate	n-Hexane	0.0250

Pressures	
Condenser Pressure	300.000 kPa
Reboiler Pressure	300.000 kPa

Reflux Ratios	
External Reflux Ratio	8.999
Minimum Reflux Ratio	7.530

Table 3: Data from Shortcut Distillation Column

Trays	
Minimum Number of Trays	30.084
Actual Number of Trays	62.269
Optimal Feed Stage	40.639

Temperatures	
Condenser [C]	99.44
Reboiler [C]	106.3

Flows	
Rectify Vapour [kgmole/h]	57.451
Rectify Liquid [kgmole/h]	51.701
Stripping Vapour [kgmole/h]	57.451
Stripping Liquid [kgmole/h]	61.272
Condenser Duty [kJ/h]	-1461603.429
Reboiler Duty [kJ/h]	1448687.118

Table 4: Data from Shortcut Distillation Column

Name	3	5	4
Vapour	1.0000	0.0000	1.0000
Temperature [C]	250.0	258.7	258.7
Pressure [kPa]	1300	1300	1300
Molar Flow [kgmole/h]	713.3	0.0000	713.3
Mass Flow [kg/h]	6.147e+004	0.0000	6.147e+004
Std Ideal Liq Vol Flow [m3/h]	93.08	0.0000	93.35
Molar Enthalpy [kJ/kgmole]	-1.281e+005	-1.456e+005	-1.281e+005
Molar Entropy [kJ/kgmole-C]	218.6	178.1	164.7
Heat Flow [kJ/h]	-9.138e+007	-0.0000	-9.138e+007

Table 5: Input Data for Distillation Column

	10	Recycle
n-Hexane	0.9328	0.9332
2-Mpentane	0.0672	0.0668

Table 6: Mole Composition of 2-Mpentane and n-Hexane for Distillation Column

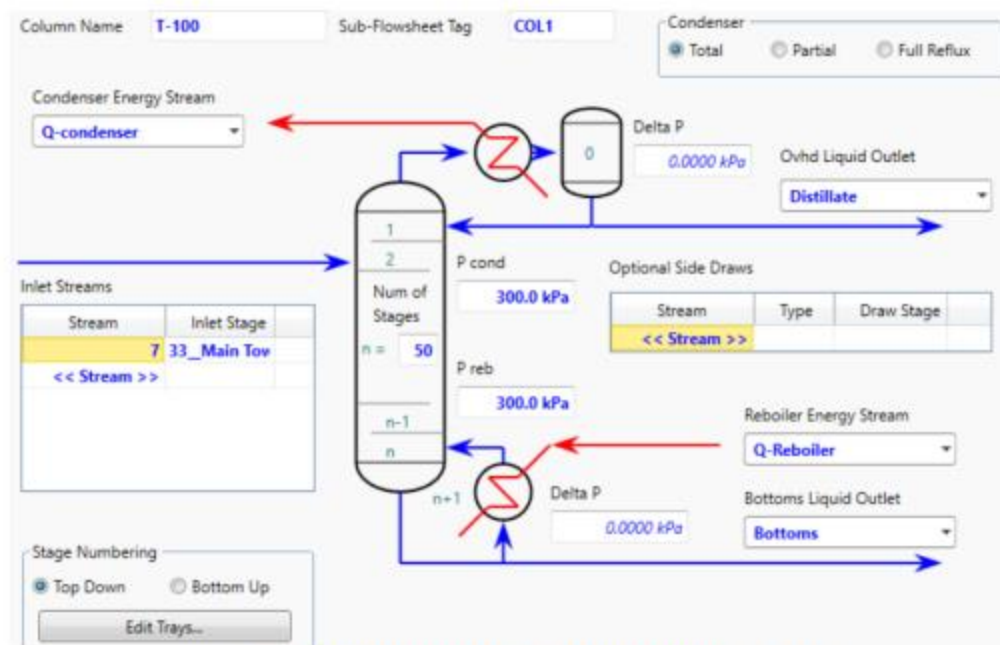


Figure 2: Detailed Components needed in Distillation Column

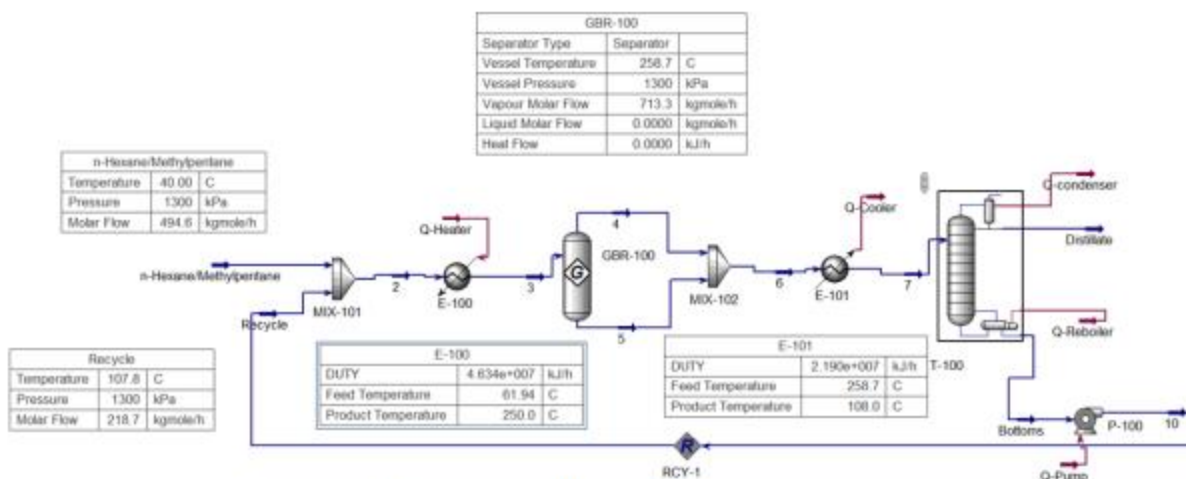


Figure 3: Isomerization Process of Naphtha Schematic

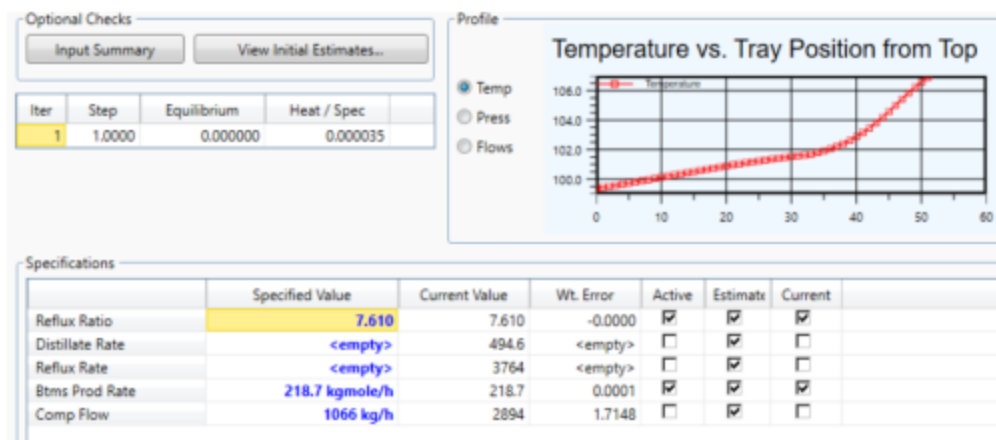


Figure 4: Temperature vs Tray Position Graph with Specifications

Recommendations for further development

During this project we hit many obstacles with the limited problem statement and no research material with subject dealing how we put in different components into ASPEN HYSYS. ASPEN has many tutorials on YouTube which we have used but for some reason our program would not run right so we just recommend that we get a more in dept tutorial of ASPEN HYSYS. This project should include pictures of final results needed because there was no way for us to know if our data was correct.

Conclusion This project was aimed to further showcase the skills we have learned in our chemical engineering courses. The isomerization of naphtha is a real world application and

by using a short cut column to extract a range of parameters to be able to fully design our complete process with a distillation column.

References

1. Zahra Ghazizahedi, Majid Hayati-Ashtiani. (2020) Retrofitting isomerization process to increase gasoline quality and decrease CO₂ emission along with energy analysis using Pinch Technology. *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects* 0:0, pages 1-12 *ZEOSOM Technology: Light Naphtha Isomerization - Iocl.com*. https://www.iocl.com/download/RND/Z_1.pdf.
2. "Explore Scientific, Technical, and Medical Research on ScienceDirect." *ScienceDirect.com | Science, Health and Medical Journals, Full Text Articles and Books.*, <https://pdf.sciencedirectassets.com/278684/>.

3. Valavarasu, G. & Sairam, B.. (2013). Light Naphtha Isomerization Process: A Review. *Petroleum Science and Technology*. 31. 10.1080/10916466.2010.504931.
4. Naqvi, Salman Raza, et al. "New Trends in Improving Gasoline Quality and Octane through Naphtha Isomerization: A Short Review - Applied Petrochemical Research." SpringerLink, Springer Berlin Heidelberg, 27 June 2018, <https://link.springer.com/article/10.1007/s13203-018-0204-y>.

AVERAGE

Average Student Original Graded Assignment

Prairie View A&M University
Roy G. Perry College of Engineering
Department: Chemical Engineering



CHEG 3305-P01
Equilibrium Stage Separation Processes
Project:
Final Project on Distillation

Due Date: 5/6/2022

Submitted By:

Shelton Amaram, Jeffrey Sanders, Isaiah Waters, Erron Williams

Submitted to: Dr. Nabila Shamim

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Executive Summary

During this project our group objective study was to design a simulation using ASPEN to determine the recycle flow rate and composition of a crude oil mixture that includes n-hexane and methyl pentane which will be input through a distillation column. A part of the objective this project will also give us more experience with using real world problems to create solutions within a simulation modeling software whilst working as a team to gather information through textbook material and connect our past course knowledge. The solutions to this project will be depicted throughout our process description and simulation results which we should notice an overall conversion of 95% achieved from the reaction. The bottom product of this distillation shall be rich in n-hexane and to be recycled to the reactor feed for a continued flow process. Within our process we assumed that the feed comes in at 1300KPa with an isobaric heater. We also assume that regular sensible heat occurs in the first heater under the same conditions listed in the problem statement.

Our project displays consistencies through the process and shows that the specified values followed within the system where accurate the rates in the distillation and bottoms came out as required outputs. The 95% achieved conversion is an accurate value depicted within the tables observed in the ASPEN software. We ran a successful simulation with a reflux ratio of 7.610 and our products produced the proper solutions to make the problem statement true. We have developed a greater understanding of the ASPEN software throughout the tenure of this project and have become more familiar with creating an algorithm to pass in this simulation. The number of trays within our distillation column came out to 50 with an optimal feed stage of 33. By doing this simulation we determined the recycle flow rate and composition of this mixture. The recycle flow rate was 218.6 kgmol/h and the composition of our two components came out as follows: n-hexane=0.6545 in liquid phase and 2-Mpentane=0.3455 in liquid phase. The ideal conditions were followed in our process and the mole fractions of each component at the specific values allowed a correct process to be converged.

Problem Statement

Light naphtha is a mixture produced by distillation of crude oil. Light naphtha primarily contains alkane compounds (paraffin), and it can be blended into gasoline. The octane value of methyl substituted alkanes (iso paraffin) is higher than that of staring chain compounds (normal paraffin), so it is often advantageous to isomerize the light naphtha to increase the proportion of branched compounds.

A simple naphtha isomerization process has a feed of 10,000 barrels per day of a 50 wt.% mixture of n-hexane and methyl pentane. The fed is heated and sent to a reactor where it is brought to equilibrium at 1300KPa and 250°C. The reactor products are cooled to the dew point and fed to a distillation column operated at 300KPa. The bottom product of the distillation is rich in n-hexane and is recycled to the reactor feed. An overall conversion of 95% is achieved.

Simulate the process to determine the recycle flow rate and composition.

Process Description

Our process design consisted of the following components in order: a mixer, heater, Gibbs reactor, a second mixer, a distillation column, a pump, and a recycler. Firstly, the feed enters the mixer with the recycled product at 40°C and 1300 kPa. At state point 2, the stream is then heated and then sent through a Gibbs Reactor for isomerization. The two product streams from the Gibbs Reactor are mixed again and then cooled to the dew point, 108°C. At state point 7, this is where the distillation process begins. The stream goes through the distillation process where distillate and bottoms products are formed. The distillate is our main product, whereas the bottoms continues through a pump. The pump allows the stream to be recycled and reentered into the cycle at a pressure consistent with the initial pressure of the feed. The entire simulation is shown in the figure below.

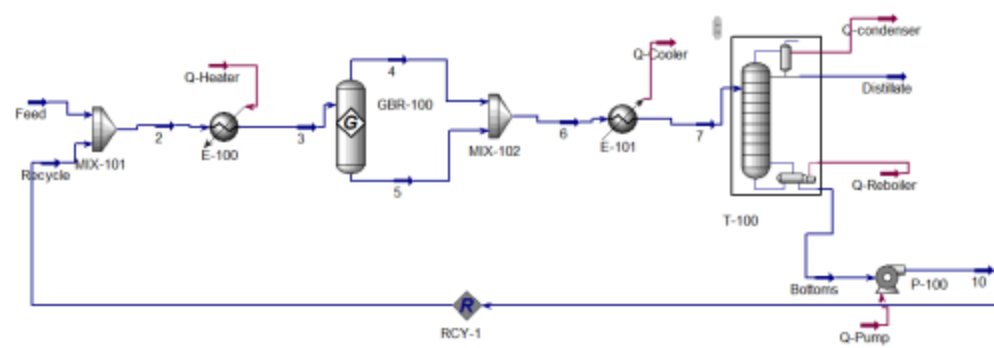


Figure 1: Rigorous Distillation Process Simulation

Process Simulation and Results

In order to solve the problem statement, we needed to follow the specifications from the problem methodically. By this we were inclined to design each unit one-by-one, making sure that each was converging successfully before proceeding. We had to familiarize ourselves with the software and understand the problem statement overall.

The feed conditions were specified in the beginning as follows: An initial feed of 10,000 Barrels/day of 50wt% n-hexane, 50wt% 2-methylpentane, at 1300 kPa and heated and isomerized at 250°C then cooled to the dew point at 300 kPa before it is fed into a distillation column. (The mass flow rate was calculated through dimensional analysis and by taking the average densities of the components into our calculations below).

$$v_o = 10000 \frac{\text{Barrels}}{\text{day}} \cdot 0.1589 \frac{\text{m}^3}{\text{barrel}} = 1589.9 \frac{\text{m}^3}{\text{day}}$$

$$\rho = \frac{(0.654g \cdot 1kg \cdot 1000mL \cdot 1000L)}{(1mL \cdot 1000g \cdot 1L \cdot 1m^3)} = 654 \frac{kg}{m^3} \cdot 654 \frac{kg}{m^3} \cdot 1589.9 \frac{m^3}{day} = 1,039,794.6 \frac{kg}{day}$$

$$1,039,794.6 \frac{kg}{day} \cdot \frac{1 day}{24hr} = 43324.78 \frac{kg}{hr}$$

Specifying the temperatures and pressures at the states in between the units allowed the software to define heat duties from the heat exchangers. We chose to set our initial feed temperature to 40C since that's the temperature at which our density is equal to 654 kg/m³. This feed then went through the heat exchanger to be brought to 250C at constant pressure before entering the Gibbs reactor. The Gibbs reactor was implemented to carry out the isomerization in our process. After leaving this reactor the mixer is responsible for bringing the components into equilibrium before feeding into our condenser. After the feed was brought to our Dew point of (108C) before entering the distillation unit.

It was necessary for us to first conduct a short-cut distillation first. The short-cut distillation simulation design is shown in Figure 2. Doing this allowed us to determine the optimal feed stage and the theoretical number of trays within the column. This was also the stage in the process where the external reflux ratio was determined. (By plugging in certain values for the column, the simulator automatically supplied us with the minimum reflux ratio. We then multiplied this number by 1.2 to find the actual reflux.) Finding this component then led to the development of our final distillation. Through these findings we were able to input the specific values of the compositions and finalize the distillate and the bottoms product.

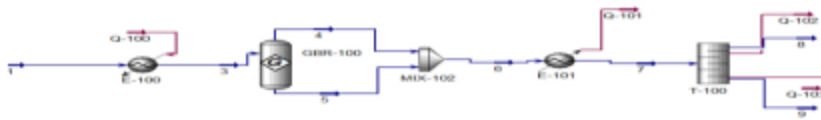


Figure 2: Simulation with Short-Cut Distillation

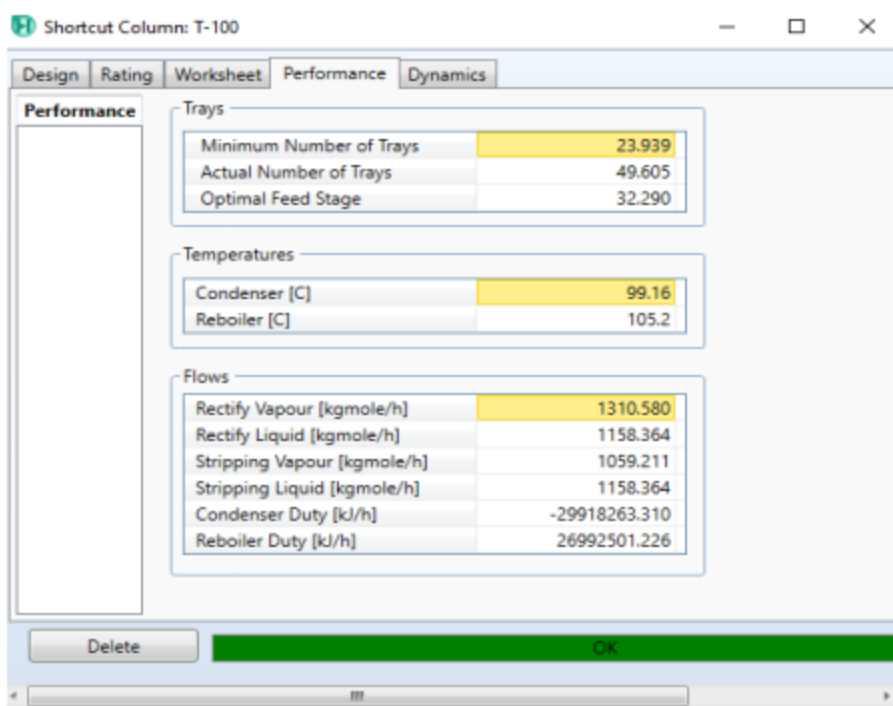


Figure 3: Short Column Performance Specifications

Once we determined the number of trays, optimum feed location, and reflux ratio in Figure 3, we were then able to apply those conditions to a Rigorous Distillation model. The distillation specifications are shown in Figure 4 below. As shown, the number of trays used was 50, and the feed was designated to enter at stage 33 (optimum feed location). This unit was to be operated under pressure conditions of 300 kPa throughout the column. Therefore, the reboiler and condenser pressure were set at that value.

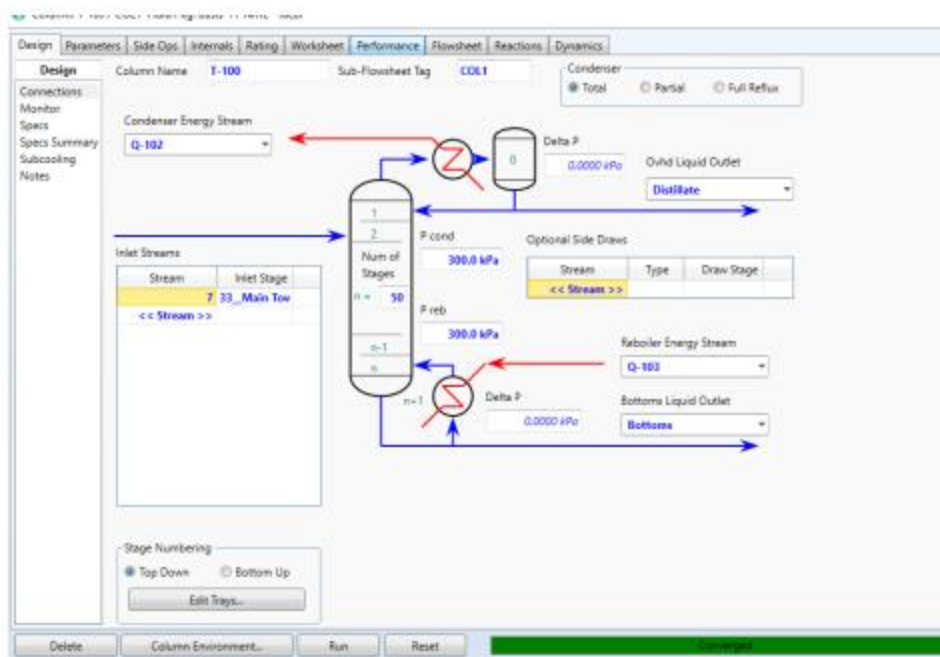


Figure 4: Distillate Specifications

After sending the bottoms feed through a pump for recycling, the compositions and flow rate were determined. The feed conditions of the product streams are shown in the figures below (bottoms, distillate, and recycle).

Material Stream: Bottoms

Worksheet Attachments Dynamics

	Mole Fractions	Liquid Phase
n-Hexane	0.6545	0.6545
2-Mpentane	0.3455	0.3455

Total 1.00000

Edit... View Properties... Basis...

OK

Delete Define from Stream... View Assay

Figure 5: Material Stream Bottoms Compositions

Material Stream: Bottoms

Worksheet Attachments Dynamics

Worksheet	Stream Name	Bottoms	Liquid Phase
Conditions	Vapour / Phase Fraction	0.0000	1.0000
Properties	Temperature [C]	103.7	103.7
Composition	Pressure [kPa]	300.0	300.0
Oil & Gas Feed	Molar Flow [kgmole/h]	218.6	218.6
Petroleum Assay	Mass Flow [kg/h]	1.884e+004	1.884e+004
K Value	Std Ideal Liq Vol Flow [m3/h]	28.53	28.53
User Variables	Molar Enthalpy [kJ/kgmole]	-1.838e+005	-1.838e+005
Notes	Molar Entropy [kJ/kgmole-C]	117.3	117.3
Cost Parameters	Heat Flow [kJ/h]	-4.019e+007	-4.019e+007
Normalized Yields	Liq Vol Flow @Std Cond [m3/h]	28.40	28.40
	Fluid Package	Basis-1	
	Utility Type		

OK

Delete Define from Stream... View Assay

Figure 6: Material Stream Bottoms Conditions

Material Stream: Distillate

Worksheet Attachments Dynamics

Worksheet

- Conditions
- Properties
- Composition
- Oil & Gas Feed
- Petroleum Assay
- K Value
- User Variables
- Notes
- Cost Parameters
- Normalized Yields

	Mole Fractions	Liquid Phase
n-Hexane	0.0515	0.0515
2-Mpentane	0.9485	0.9485

Total 1.00000

Edit... View Properties... Basis...

OK

Figure 7: Material Stream Distillate Compositions

Material Stream: Distillate

Worksheet Attachments Dynamics

Worksheet	Stream Name	Distillate	Liquid Phase
Conditions	Vapour / Phase Fraction	0.0000	1.0000
Properties	Temperature [C]	99.30	99.30
Composition	Pressure [kPa]	300.0	300.0
Oil & Gas Feed	Molar Flow [kgmole/h]	251.4	251.4
Petroleum Assay	Mass Flow [kg/h]	2.166e+004	2.166e+004
K Value	Std Ideal Liq Vol Flow [m3/h]	32.98	32.98
User Variables	Molar Enthalpy [kJ/kgmole]	-1.882e+005	-1.882e+005
Notes	Molar Entropy [kJ/kgmole-C]	-3.763	-3.763
Cost Parameters	Heat Flow [kJ/h]	-4.730e+007	-4.730e+007
Normalized Yields	Liq Vol Flow @Std Cond [m3/h]	32.89	32.89
	Fluid Package	Basis-1	
	Utility Type		

OK

Delete Define from Stream... View Assay

Figure 8: Mateial Stream Distillate Conditions

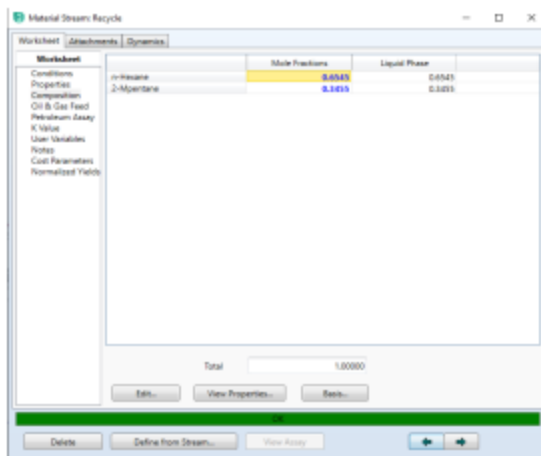


Figure 9: Material Stream Recycle Compositions

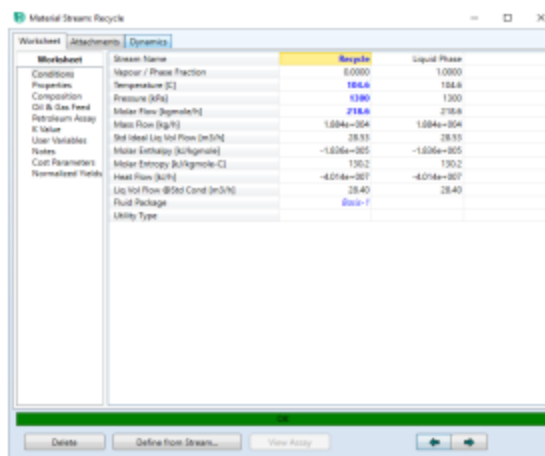


Figure 10: Material Stream Recycle Conditions

As shown in Figures 9 and 10, we successfully completed the problem by solving for the recycle stream flow rate and compositions. For the flow rate, it was determined to be **218.6 kgmol/h**, and the compositions were **0.6545 for n-Hexane** and **0.3455 for 2-methylpentane**.

Recommendations for further development

One recommendation that would be beneficial for the future would be to try to do a similar type of simulation beforehand using a tutorial so the group would not be trying to figure out how to do the simulation at the same time as it is due. That way the project would have gone smoother. Multiple simulations would give the group a greater sense of security in knowing that the project could be completed. With all these tasks being accomplished, the result of a more efficient simulation process would be achieved at a higher rate than it did this time.

Conclusions

In conclusion, with the help of ASPEN HYSYS we were able to further our understanding of the distillation process of binary systems. In this process we also had to test our knowledge of Thermodynamics in making sure that the conditions of the feeds left each unit lined up with the desired specifications needed to reach our optimal product. Overall, our team feels more prepared knowing that we can now create a multi-unit system in ASPEN.

References

<https://pubchem.ncbi.nlm.nih.gov/compound/3-methylpentane?msclid=dc9db893cdbf11ec9740ae1547d988fb>

[N-HEXANE](#) | [CAMEO Chemicals](#) | [NOAA](#)

[Distillation Column - an overview](#) | [ScienceDirect Topics](#)

BELOW AVERAGE

Below Average Student Original Graded Assignment

Prairie View A&M University

Roy G. Perry College of

Engineering Department:

Chemical Engineering



CHEG 3305

Equilibrium Stage Separation Processes

Distillation

Final Project

Due Date: May 6, 2022

Britton Andrews

Ariel Kinsey

Isis Solomon

Maya Spears

Submitted to: Nabila Shamim

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Table 2: Case – Material System

Executive Summary

Gasoline is a mixture of hydrocarbons with many branches needed to lubricate an engine to prevent 'knocking,' which makes the isomerization of light naphtha ideal. In this process, crude oil is distilled to produce light naphtha. The octane value, a fuel's ability to prevent 'knocking' when light, increases during this process. The octane value of isoparaffin or methyl-substituted alkanes is greater than the starting chain, normal paraffin.

In this simulation, it was required to design the isomerization process of light naphtha in ASPEN HYSYS with a final conversion of 95%. The problem statement was as follows:

A mixture of 50 wt. % of n-hexane and methyl pentane at 10000 barrels a day is heated and sent to a reactor. The mixture is brought to equilibrium at a pressure of 1300 kPa and a temperature of 25°C. Once the product leaves the reactor, the product is cooled to the dew point of the mixture. The mixture is then fed into a distillation column with an operating pressure of 300 kPa. Rich n-hexane is the product at the bottom of the distillation column and is then recycled back into the reactor.

The objective of this project, after designing the process, is to generate the recycle stream values, flow rates, and composition values.

Process Description

An Aspen HYSYS simulation is run utilizing the Peng-Robinson model to start the process. The two components, n-hexane, and methyl pentane were entered into the program. After the components were entered, a mixer was placed on mixing the two streams to begin building the simulation. After leaving the mixer, the stream heads into the heater to increase the temperature before heading into the Gibbs Free Reactor.

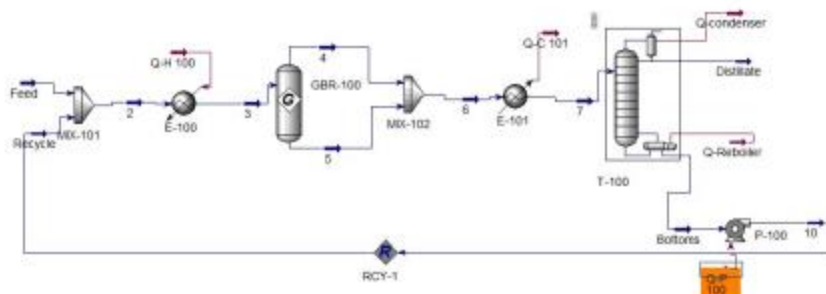


Figure 1: Isomerization of Light Naphtha Process

After leaving the Gibbs Free Reactor, the stream is cooled into the distillation column at its dew point properties. The bottom stream is then pumped to the recycle stream while the distillate stream exits the system. The bottom stream is then recycled back through the entire system, starting the process once again. The initial temperature is assumed to be 50 degrees Celsius to keep the stream in the liquid phase since the boiling points of n-hexane and methyl pentane is 69 degrees Celsius and 60 degrees Celsius, respectively. The mole fraction for the light key (methyl pentane) is assumed to be 0.2000 in the bottoms. The mole fraction for the heavy key to distillate (n-hexane) is then calculated to be 0.0250. The condenser pressure is assumed to be 4 atm, and the re-boiler pressure is 6. The external reflux ratio is then chosen to be 7.

Process Simulation and Results

After simulating the process in Aspen HYSYS, the objective of the project was met. The recycle stream values were found, as well as the compositions and flow rates. The results are shown below.

	Unit	3	Feed	4	5	6	7	Distillate	Bottoms	Recycle	10	2
Comp Mole Frac (n-Hexane)		0.58238	0.5	0.33219	0.35356	0.33219	0.33219	0.05186	0.68655	0.68665	0.68655	0.58238
Comp Mole Frac (2-Mpentane)		0.41762	0.5	0.66781	0.64644	0.66781	0.66781	0.94814	0.31345	0.31335	0.31345	0.41762

Table 1: Component Composition

After putting in the assumed and known values, HYSYS calculated the minimum reflux ratio.

The external ratio was calculated by using a factor of 1.2 times higher than the minimum. The

value calculated is 7.610. Once the reflux ratio was calculated, Aspen gave an estimated

value of trays needed which was 50 and the feed stream coming in at tray number 25. Aspen

then generated a Material Stream table, which is shown below. Table 2 gives the value of the

re-boiler heat input. The value calculated is $-183,933 \frac{kJ}{kgmole}$.

Name	3	Feed	4	5	6	7	Distillate	Bottoms	Recycle	10	2
Pressure [kPa]	1300	101.3	1300	1300	1300	300	300	300	1300	1300	101.3
Temperature [C]	250	50	257.311398	257.311398	257.311398	108	99.2976821	103.999661	104.870518	104.869147	64.6975016
Mass Flow [kg/h]	42671.8355	23838.1748	42671.8355	0	42671.8355	42671.8355	23824.1771	18847.6556	18833.6607	18847.6556	42671.8355
Std Ideal Liq Vol Flow [m ³ /h]	64.6465841	36.1419312	64.7976766	0	64.7976766	64.7976766	36.2718101	28.5258623	28.5046529	28.5258623	64.6465841
Vapor / Phase Fraction	1	0	1	0	1	1	0	0	0	0	0.07779965
Molar Enthalpy [kJ/kgmole]	-128442.82	-196277.73	-128442.82	-145989.53	-128442.82	-158814.86	-188169.58	-183549.17	-183348.04	-183348.94	-190571.08
Utility Type											
Stream Price											
Stream Price Basis	Molar Flow	Molar Flow	Molar Flow	Molar Flow	Molar Flow	Molar Flow	Molar Flow	Molar Flow	Molar Flow	Molar Flow	Molar Flow
Cost Rate [Cost/s]											

Table 2: Case – Material System

Recommendation

An extensive recommendation cannot be concluded because the required software to analyze the cost of the component streams listed in table 2 is unavailable. Therefore, it is our recommendation to complete the simulation again with the correct software.

Conclusions

In Aspen HYSYS, a model distillation process was created using the Peng-Robinson package. The goal of this simulation was to create and find the composition information, recycle stream values, and the different flow rates needed to make the process run efficiently. After the process was made and ensured to run properly, Aspen was able to calculate the needed values which can be seen in the results section. Since the cost information was not able to be generated, there was no substantial recommendation for the future. However, another group could run this same simulation once the cost information is able to be given and supply a recommendation.

References

Geankoplis, Christie J. *Transport Processes and Separation Process Principles*. Pearson, 2020.