

BINDER FOR OUTCOME "1"

*"An ability to identify, formulate, and solve complex engineering problems
by applying principles of engineering, science, and mathematics."*

**COLLEGE OF ENGINEERING
CHEMICAL ENGINEERING DEPARTMENT
PRAIRIE VIEW A&M UNIVERSITY**

**BINDER CONTAINING REPRESENTATIVE
ASSIGNMENTS FROM ALL COURSES USED TO
ASSESS OUTCOME "1"**

Last 4 Academic Years

09/10/2021 Revision

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 - CHEG 3043 Equilibrium Stage and Separation Processes**
 - CHEG 3063 Chemical Reaction Kinetics and Reactor Design**
 - CHEG 4033 Process Dynamics and Control**

2. Description of Outcome "1" and its Performance Criteria

Outcome 1:

An ability to identify, formulate and solve complex engineering problems by applying the principles of engineering, science, and mathematics

Sub-Outcomes and Performance Criteria

- 1.1: Identify & Formulate CEP (i-vi) based on Engineering , Science , and Mathematics
- 1.2: Solve CEP (i-vi) based on Engineering , Science , and Mathematics

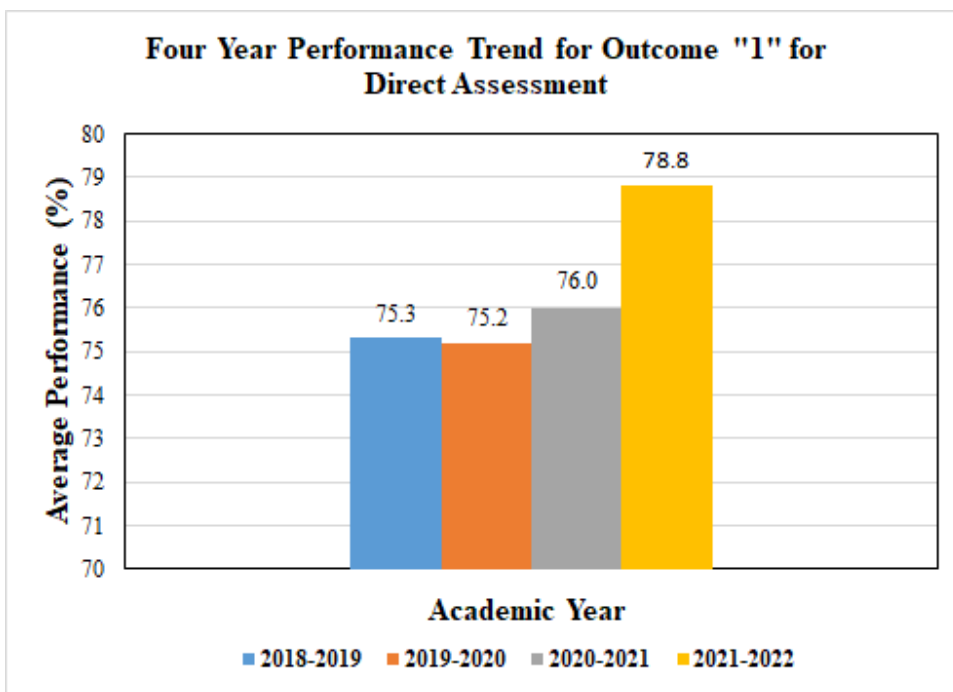
3. List of Courses Used to Assess the Outcome

Outcome 1 is assessed in the following courses:

- CHEG 3043 Equilibrium Stage and Separation Processes
- CHEG 3063 Chemical Reaction Kinetics and Reactor Design
- CHEG 4033 Process Dynamics and Control

4. Summary Assessment Results and Continuous Improvements for Outcome “1” over the Assessment Years.

The average performance for all students in the 3 courses used to assess outcome 1 for the past Four academic years are shown below



Problems identified and recommended actions to be taken to address problems

1. At the course level

Problems Identified in the Various Courses	Recommended Actions to be Taken	Basis for Action
1. Student sometimes still attempted problem solving without proper use of identify and formulate steps. 2. Inability to do analysis on software. A new version of ASPEN delayed the interpretation of the assignment. 3. Students could not conceptualize, identify the physical laws, and analyze problems that are different from an example problem they have seen before 4. Student inability to identify control variables, constraint, and formulate material and energy balance equation needed to solve a chemical engineering problem	1. Promulgate active learning in class and continue assignments with collaborative learning. 2. Continue with activities that introduce simulation software like Aspen/HYSYS and effective use of Excel spreadsheets. Include high quality handouts that will clearly describe the procedure for using of these tools and how to interpret the data generated by these tools. 3. In keeping with using the simulation tools, instructors should give smaller assignments that build to the final design project using HYSYS. 4. The instructor should give students a grading rubric, which highlights the importance of the actual data interpretation process. 5. More tutoring is needed, TA for higher level classes are required. Instructor can work one to one with student and can be more involved. 6. Discuss more scenarios and give more course assignments.	Though the expected target average for student performance was met but , the aggregate percentage of student meeting the expected average was 62 % which is below our set target of 70 %

2. At Department Level

(1) Faculty members in the program met periodically to review data from the Program Outcome Assessment Reports. The weak areas of outcomes performance were identified. Perceived problems were discussed in this forum. Faculty were provided with the data collected from student exit surveys for their review, as well as input from the Industrial Advisory Council (IAC).

(2) Introduction of a new 2-credit hour course CHEG 1022, Introduction to Computations in CHEG, which will be taught in the spring semester of the freshman's year. CHEG 1022 will be an introductory course of important chemical engineering concepts and computations. Students will learn how to classify problems based on their mathematical nature. Topics include basic introductory calculation involving material and energy balances, fluid flow phenomena, fundamental thermodynamics and kinetics, and introductory software and simulation tools such as Visual Basic and CHEMCAD. This new course (CHEG 1022) will ensure our students acquire the skills needed in subsequent courses. The new course will build on our revamped and re-organized course CHEG 1021, Introduction to Chemical Engineering, and will be a pre-requisite for CHEG 2053, Material & Energy Balances.

(3) An additional program-level action that resulted from faculty consideration of exit survey findings to address teaching quality is the introduction of teaching observation of an instructor by fellow department colleagues

Basis of Action:

The students' performance average for Outcome 1 in the last three academic cycles (2018-2019, 2019-2020 and 2020-2021) met the target average of 75%. However, the aggregate percentages of students (66 % and 62 %) meeting the expected average in the previous two academic cycles

(2018-2019) were below the set target of 70 % except for the last academic cycle (2020-2021/ 72.5 %) which exceeded the set target. The reason for this improvement could largely be due to the implementation of a significant portion of the recommended actions both at the course and departmental levels in the last academic cycle (2020-2021).

6. Sample Assignments and Justification of suitability of assignment for measuring the outcome in :

CHEG 3043 Equilibrium Stage and Separation Processes

CHEG 3063 Chemical Reaction Kinetics and Reactor Design

CHEG 4033 Process Dynamics and Control

**OUTCOME “1” SPECIFIC ASSIGNMENTS
USED TO ASSESS THE OUTCOME IN
SEPARATION PRCESS**

**Note: This section needs to be repeated for the other
courses in which outcome "1" is assessed.**

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
EQUILIBRIUM STAGED SEPARATION PROCESSES
SPRING 2021**

Instructor: Irvin W. Osborne-Lee

Title of Assignment

PROJECT 1 - *Flash and Flash Cascade Separation Design*

Outcome Measured Using this Assignment

Outcome 1

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

Check the complex engineering problem characteristics related to this assignment

Assignment problem	
	involves wide-ranging or conflicting technical issues,
X	has no obvious solution
	Addresses problems not encompassed by current standards and codes
	involves diverse groups of stakeholders
X	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
X	science
X	mathematics

Brief justification of why this assignment is suitable for this outcome

The design tasks lead to an open ended solution and involve an inter-related set of steps that require the student to employ math skills, knowledge of science including thermodynamics, and engineering concepts. Students must demonstrate understanding of phase equilibrium, ability to use material and energy balances, and skills with graphical methods and chemical process simulation.

Rubric for Grading Letter Report for Project 1: Flash and Cascade Design & Simulation

Task Description: This assignment is a collaborative learning assignment. Work in teams assigned. Teams may consult each other but each team must prepare a project results poster presentation in Powerpoint™ and submit a letter report done up in Word.

Criteria	weight	Excellent 4 Yes	Good 3 Yes, but	Fair 2 No, but	Unacceptable 1 No
Format	10%	☒ Directly relevant to letter report style	☐ Somewhat relevant to letter report style	☐ Remotely related to letter report style	☐ Totally unrelated to letter report style
Organization	10%	☒ Good organization; points are logically ordered; sharp sense of beginning and end	☐ Organized; points are somewhat jumpy; sense of beginning and ending	☐ Some organization; points jump around; beginning and ending are unclear	☐ Poorly organized; no logical progression; vague beginning and ending
Quality of Information	25%	☒ Supporting details specific to subject; figures and tables captioned, called out and well discussed	☐ Some details are non-supporting to the subject; figures and tables captioned, called out and discussed	☐ Details somewhat sketchy; do not support topic. Not all figures/ tables captioned, called out and discussed	☐ Unable to find specific details. Figures and tables not captioned, called out and discussed
Grammar, Usage, Mechanics, Spelling	25%	☒ No errors	☐ Only one or two errors	☐ More than two errors	☐ Numerous errors distract from understanding
References	10%	☒ Citations are used wherever needed and helpful; are called out and organized properly.	☐ Citations are used in most places where needed; are mostly called out and organized properly.	☐ Citations are sometimes used but are not consistently called out and organized properly.	☐ Citations are not used or are used improperly.
Neatness	10%	☒ Typed; clean; neatly bound in a report cover; illustrations provided	☐ Legible writing, well-formed characters; clean and neatly bound in a report cover	☐ Legible writing, some ill-formed letters, print too small or too large; papers stapled together	☐ Illegible writing; loose pages
Timeliness	10%	☒ Report on time	☐ Report one class period late	☐ Report two class periods late	☐ Report more than one week late

Assignment Score

100

McIntyre/Osborne-Lee

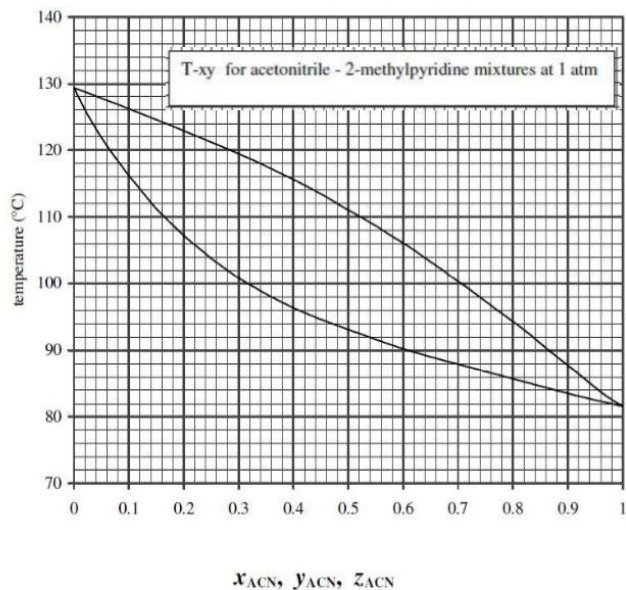
Exemplary work!

Flash and Flash Cascade Separation Design Project

This assignment is a collaborative learning assignment. Work in teams assigned (see Table 1). Teams may consult each other but each team must prepare a project results poster presentation¹ in Powerpoint™ and submit a letter report² done up in Word™. It is proposed to use a two-unit flash distillation *cascade* to separate a binary mixture of Component A and Component B. The feed stream to the first unit is has a mole fraction given by Z_A . Both separators are operating at P_O . Answer the design questions below.

- If the first unit operates at T_1 , what stream amounts and compositions will be produced and what fraction of the feed stream is vaporized in the first step of the process?
- If the vapor produced in the first unit is fed to the second unit, what should the operating temperature T_2 be to vaporize a fraction of the feed (given by f_2) of the feed to the second unit?
- What product streams and compositions are achieved for the cascade overall?
- How many units N are needed in a cascade to achieve a product stream with 95% purity for the light key?
- For parts (c) and (d) above, compare your findings using the graphical methods with results from simulation using modeling software such as AspenHYSYS.

VLE data for a sample binary system at 1 atm is provided in the table below. You must obtain the data for your *particular* system (see Table 1).



¹ The rubric showing the grading criteria for oral or video presentations is published at the eCourse site for this course.

² The format for the letter report is given in a sample report published at the eCourse site for this course.

	Name of Team Members	Team Number	Component A	Component B	Feed Comp. Z_A	Op. Temp.. T_1	Frac. Vap'd. f_2	Prod. Purity %
1	Alexander, Cayla	1	Water	2-methyl-1-butanol	0.3	120°C	0.33	93
2	Livingston, Ryan	1						
3	Anaghara, Ike	2	Isopropanol	3-methyl-1-butanol	0.4	107°C	0.4	92
4	Lovelace, Alexis	2						
5	Atatah, Irene	3	1-Propanol	2-methyl-1-butanol	0.35	119°C	0.5	94
6	Mahmood, Wasil	3						
7	Barnes, Zsamia	4	Ethanol	3-methyl-1-butanol	0.2	111°C	0.6	95
8	Marshall, Bryson	4						
9	Butler, Dayna	5	Ethanol	2-methyl-1-butanol	0.15	123°C	0.67	96
10	Nkemadu, Chioma	5						
11	Franklin, Tyecia	6	Methanol	2-Propanol	0.45	75°C	0.45	90
12	Ukpede, Laura	6						
13	Henderson, Ebonie	7	Methanol	1-Propanol	0.13	93°C	0.25	94
14	Vaughn, Cherish	7						
15	Asfaha, Kibrom	8	Methanol	2-butanol	0.22	91°C	0.75	93
16	Williams, Fredrick	8						

Simulation software is accessible using VDI, the Virtual Desktop Interface, and is accessible using information at this link: <https://www.pvamu.edu/its/vdi/>. Using the Windows flag button on the taskbar, scroll down to the AspenTech folder, which contains links to start Aspen and also HYSYS, both of which are chemical process simulators that the CHEG Department has licensed for your use. An open source process simulator is also available (DWSIM), which can be useful when PV systems are down. DWSIM is available at <https://dwsim.inforside.com.br/new/> (active as of 2/11/2021).

Guidance on using HYSYS is available in a paper by Hamid.³ Various video tutorials can be found on YouTube. Each student team should schedule meetings with the instructor as needed for guidance to get started and avoid staying stuck for any reason.

³ Hamid, M., An Introduction to Chemical Engineering Simulation. Available for download at eCourse site.

Sunday, 28 February 2021

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Dr. Osborne-Lee
CHEG 3043 Y01
VIA Canvas Upload

SUBJECT: Letter Report - Project 1- Flash Cascade Using Ethanol & 3-Methyl-1-Butanol

Dear Sir:

I am writing in regards to the course assignment posted to Canvas: *Upload letter report with Project 1 Findings*. The assignment was given with instructions in five points listed below.

- If the first unit operates at T_1 , what stream amounts and compositions will be produced and what fraction of the feed stream is vaporized in the first step of the process?
- If the vapor produced in the first unit is fed to the second unit, what should the operating temperature T_2 be to vaporize a fraction of the feed (given by f_2) of the feed to the second unit?
- What product streams and compositions are achieved for the cascade overall?
- How many units N are needed in a cascade to achieve a product stream with 95% purity for the light key?
- For parts (c) and (d) above, compare your findings using the graphical methods with results from simulation using modeling software such as AspenHYSYS.
 - (Note: DWSIM was used as we did not have access to AspenHYSYS.)

Distillation, a common separation process, is an essential industry process. As a reference, *Transport Processes and Separation Process Principles* by C. J. Geankoplis, was used as guidance while completing the design project. Flash distillation occurs when a binary mixture of two or more components are separated using constant temperature and pressure to establish a vapor liquid equilibrium. This results in the separation of the mixture into vapor and liquid product streams¹. In vapor-liquid systems, the component with the higher boiling point is known as the heavy key and the component with the lighter boiling point is considered to be the light key¹. The more volatile component has the lower boiling point and moves to the top of the distillation column or separation unit¹. The more volatile component also has a higher vapor pressure. The vapor stream is composed of a higher concentration of the lighter key while the liquid stream is composed of a higher concentration of the heavy key¹. Flash drums are often

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek. *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM, *Property Package Selection*. (last edited August 23, 2020). Last accessed February, 25, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

³ MK Abd Hamid, *HYSYS®: An Introduction to Chemical Engineering Simulation* (Skudai: 2007). Last accessed February, 25 2021 at http://eprints.utm.my/id/eprint/3030/2/HYSYS_for_UTM_Degree++_Program.pdf

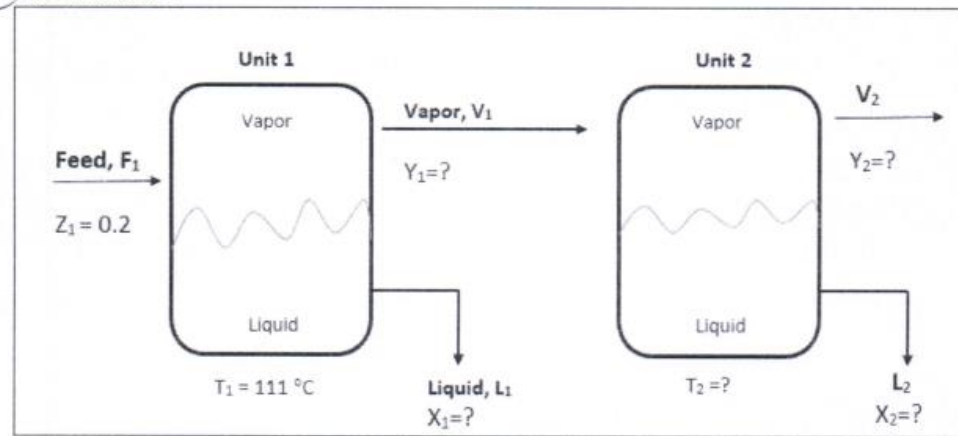
used in distillation processes. To obtain a higher purity of the light key, multiple flash drums or separation units may be utilized¹. This is known as a cascade.

Methodology

Identify

A sketch was constructed identifying the information that was given and variables that we needed to solve for. This sketch can be seen below in Figure 1. Our feed stream consists of ethanol and 3-methyl-1-butanol. The feed composition, z_i , was given as 0.2. The molar flow rates of the feed, vapor and liquid streams for each unit were to be determined along with the compositions of each stream. The operating temperature of 111°C, was given, however the operating temperature for unit 2 needs to be determined.

Figure 1. Annotated sketch used to identify the given information and the unknowns that remain to be determined



Formulate

In order to calculate the feed and product streams, we would require the use of the Inverse Lever Arm Rule or ILAR. The formulas are listed below.

ILAR:

$$V^{\wedge} = V/F = OD/BD$$

$$OD = z_i - y_i \rightarrow \text{Component } i \text{ in vapor fraction}$$

$$BD = x_i - y_i \rightarrow \text{Overall component } i \text{ balance}$$

$$F = V + L$$

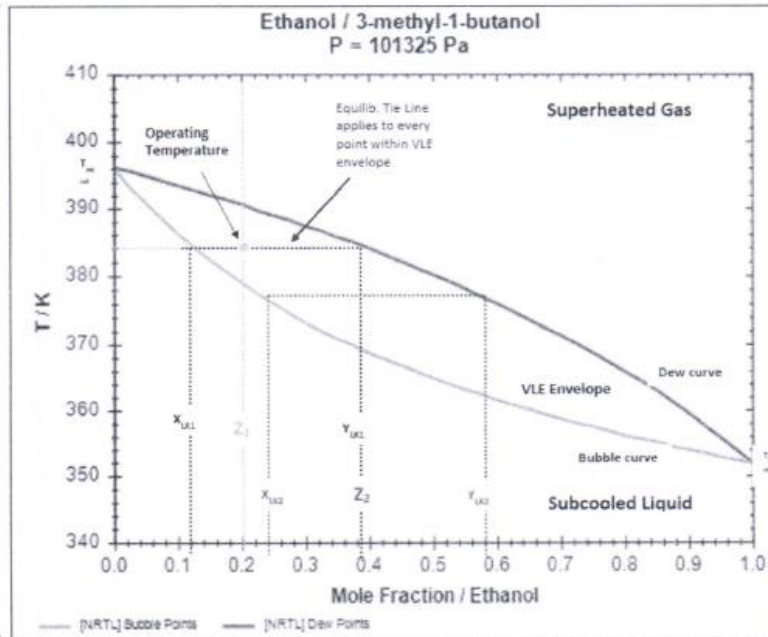
Analysis

Part A

As seen in Figure 2, DWSIM software was used to generate a Txy diagram for our light key and heavy key components at the operating temperature T_1 . The package was selected based on the

characteristics of our feed components. Detailed guidance was found on the package selection help page in DWSIM² and in the published work on HYSYS by Hamid³. The NRTL package was selected because we have polar components that are not considered to be electrolytes. To determine the compositions of the vapor stream, V_1 , and liquid stream, L_1 , the Txy diagram was used. The feed composition, z_1 , was drawn through the VLE region. The operating temperature, $T_1 = 384$ K, was used to draw an equilibrium tie line between the dew curve and bubble curve. The temperature intersected the line of the feed composition. This region was determined to be our operating point. The point on the bubble curve that fell onto that equilibrium tie line represents the composition of our light key in the liquid phase, $x_{LK,1} = 0.12$. The point on the dew curve that fell onto the equilibrium tie line represents the composition of our light key in the vapor phase, $y_{LK,1} = 0.38$. To find $x_{HK,1}$ and $y_{HK,1}$ the compositions for the light key were subtracted from one because all mole fractions add up to one. Assuming a molar flow rate of 100 kmol/hr for the feed stream, F_1 , we were able to calculate the molar flow rates for the product streams by using ILAR as seen in the Calculations section.

Figure 2. Txy Diagram generated using DWSIM Software with annotations for VLE system.



Part B

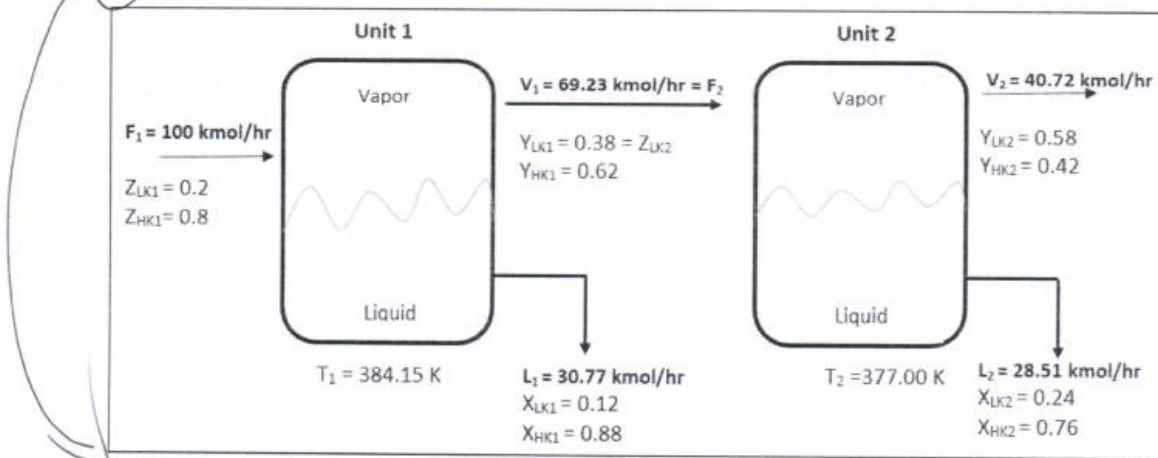
In order to determine the temperature that would vaporize a fraction of the feed to the second unit, we plotted z_2 on the Txy diagram. The vapor produced from the first unit becomes the feed

for the second unit and the composition of the more volatile component in the vapor phase equates to the feed composition, $y_{LK1} = z_2$. Various temperatures that intersected with z_2 inside the VLE region were selected as a starting point. Compositions at the corresponding temperatures were then used in ILAR to determine which values would produce a V/F ratio of 0.6. The procedure can be seen in the Calculations section. Those compositions were $x_{LK2} = 0.24$ and $y_{LK2} = 0.588$. The final operating temperature selected for unit 2 was 377.00 K.

Part C

The molar flow rates and compositions, which are displayed below in Figure 3, for the two unit cascade were found as previously discussed in Part A. Compositions were found using the operating temperature found in Part B, $T_2 = 377.00$ K. Those compositions were then plugged into equations required for ILAR, as seen in the Calculations section. The molar flow rate for the feed, which was equal to the vapor flow rate from unit 1, was used to find the molar flow rates for the product streams.

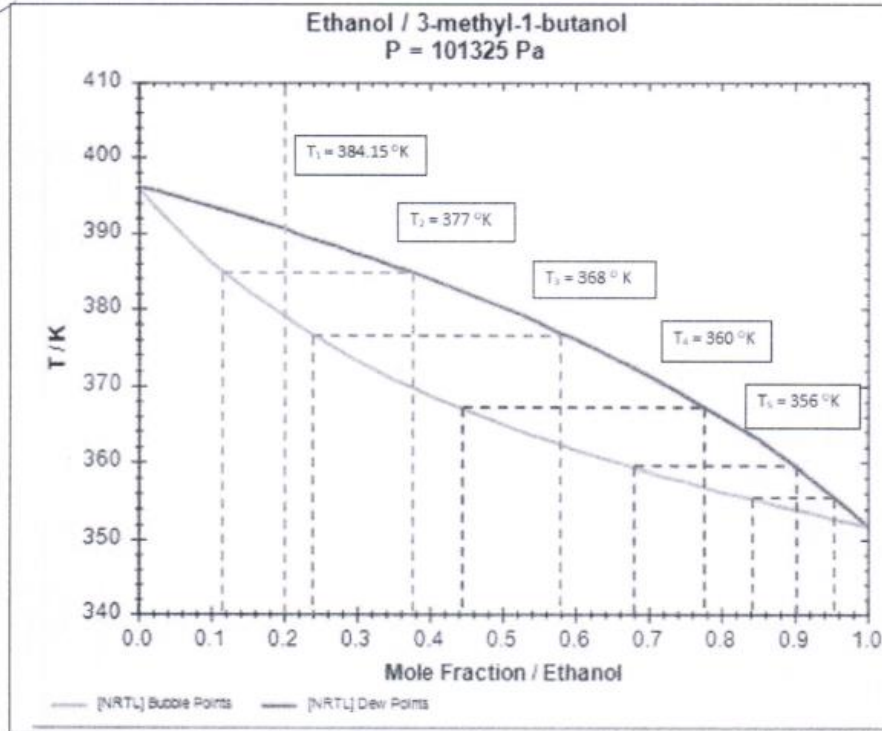
Figure 3. Annotated sketch of two unit cascade including flow rates and compositions for all streams



Part D

To find the number of units, N , that are required to produce 95% purity for the light key in the product stream, the Txy diagram was used. An additional unit was designed for a different operating temperature until y_{LK} was equal to 0.95. Each operating temperature selected within the VLE region in order to assure separation. In total, five units, $N=5$, were predicted to produce a product stream with 95% purity for the lightkey. The cascade can be seen on a Txy diagram in Figure 4.

Figure 4. Txy Diagram generated using DWSIM Software showing the needed units and the operating temperature to achieve 95% purity for the light key



Excellent work!

Part E

A simulation of the design was created in DWSIM and can be seen below in Figure 5. The operating temperature and pressure for each unit was adjusted using a series of compressors and coolers. The graphical findings are very similar to the results from the simulation obtained in DWSIM. The properties and compositions of each stream can be seen below in Table 1 and Table 2, respectively. Graphical product stream compositions differ by 0.01-0.1 with the compositions obtained from the simulation. Our molar flow rates calculated via ILAR did differ from those of the simulation. This was most likely due to an error when entering the molar flow rate of the feed and could have been a result of not pressing enter after selecting the desirable units.. Overall, the actual purity obtained from the simulation was found to be 0.948 or 94.8%.

Figure 5. Simulation results showing the streams, separation units, compressors, and coolers used in the design via DWSIM

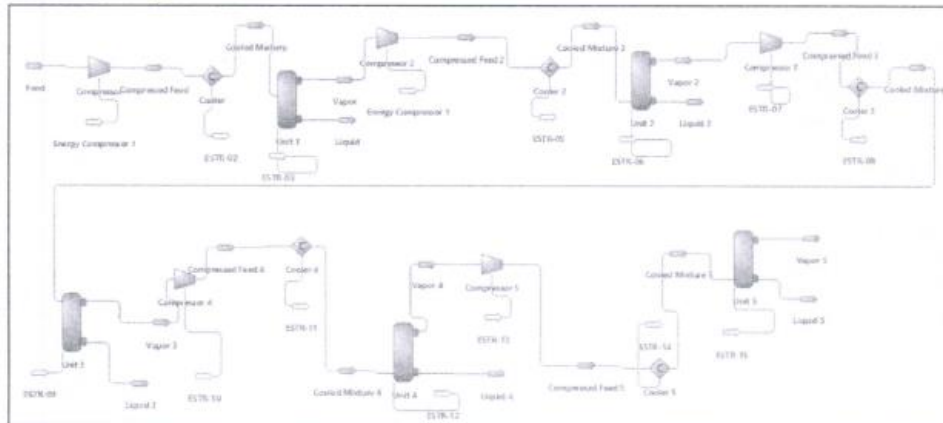


Table 1. Properties of the feed and product streams for the overall cascade simulation including temperature, pressure, molar flow rates and molar enthalpy

Property Table									
Object	Feed	Cooled Mixture	Vapor	Liquid	Cooled Mixture 2	Vapor 2	Liquid 2	Cooled Mixture 3	Units
Temperature	111	111	111	111	103.85	103.85	103.85	94.8574	C
Pressure	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	bar
Molar Flow	1.25418	1.25418	0.347663	0.906512	0.347663	0.163139	0.184324	0.163139	kmol/h
Molar Enthalpy (Mixture)	-19399.1	-19399.2	9654.5	-30536.2	-13534.5	7708.15	-32315.4	-15800.7	kJ/kmol
Object	Vapor 3	Liquid 3	Cooled Mixture 4	Vapor 4	Liquid 4	Cooled Mixture 5	Vapor 5	Liquid 5	Units
Temperature	94.8574	94.8574	86.8574	86.8574	86.8574	82.8574	82.8574	82.8574	C
Pressure	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	bar
Molar Flow	0.0751878	0.0879512	0.0751878	0.0342394	0.0409484	0.0342394	0.0210146	0.0132248	kmol/h
Molar Enthalpy (Mixture)	5794.43	-34262	-17260	4477.9	-35436.3	-11355.6	3926.54	-35639.3	kJ/kmol

Table 2. Compositions of the feed and product streams for the overall cascade simulation for each component in the mixture

Composition Table								
Object	Feed	Cooled Mixture	Vapor	Liquid	Cooled Mixture 2	Vapor 2	Liquid 2	Cooled Mixture 3
Molar Fraction (Mixture) / Ethanol	0.2	0.2	0.39408	0.12556	0.39408	0.577158	0.232218	0.577158
Molar Fraction (Mixture) / 3-methyl-1-butanol	0.8	0.8	0.60592	0.87444	0.60592	0.422842	0.767782	0.422842
Object	Vapor 3	Liquid 3	Cooled Mixture 4	Vapor 4	Liquid 4	Cooled Mixture 5	Vapor 5	Liquid 5
Molar Fraction (Mixture) / Ethanol	0.763282	0.418045	0.763282	0.894016	0.653969	0.894016	0.948919	0.806774
Molar Fraction (Mixture) / 3-methyl-1-butanol	0.236718	0.581955	0.236718	0.105984	0.346031	0.105984	0.0510812	0.193226

Make
appendix

Calculations The following calculations were used in the design of the project.

For Unit 1 - Part A

- $1 - x_{LK1} = 1 - 0.12 = 0.88 = x_{HK1}$
- $1 - y_{LK1} = 1 - 0.38 = 0.62 = y_{HK1}$
- $OD = z_1 - y_{LK1} = 0.38 - 0.20 = 0.18$
- $DB = y_{LK1} - x_{LK1} = 0.38 - 0.12 = 0.26$
- $(OD/DB) \cdot F = V \quad (0.18/0.26) \cdot 0.2 = 0.138$
- $L = F - V = 0.20 - 0.138 = 0.0615$
- $V^{\wedge}: V^{\wedge} = V/F = OD/DB = 0.18/0.26 = 0.6923$
- $V: V = V^{\wedge} \cdot F = 0.6923(100 \text{ kmol/hr}) = 69.23 \text{ kmol/hr} = V_1$
- $L = F - V = 100 - 69.23 = 30.77 \text{ kmol/hr} = L_1$

For Unit 2 - Part B

- $1 - x_{LK2} = 1 - 0.24 = 0.76 = x_{HK2}$
- $1 - y_{LK2} = 1 - 0.58 = 0.42 = y_{HK2}$
- $OD = z_2 - y_{LK2} = 0.58 - 0.38 = 0.20$
- $DB = y_{LK2} - x_{LK2} = 0.58 - 0.24 = 0.34$
- $(OD/DB) \cdot F = V \quad (0.20/0.24) \cdot 0.38 = 0.223$
- $L = F - V = 0.38 - 0.223 = 0.157$
- $V^{\wedge}: V^{\wedge} = V/F = OD/DB = 0.20/0.34 = 0.588$
- $V: V = V^{\wedge} \cdot F = 0.588(69.23 \text{ kmol/hr}) = 40.72 \text{ kmol/hr} = V_2$
- $L = F - V = 69.23 - 40.72 = 28.51 \text{ kmol/hr} = L_2$
- $V/F = 0.6 \rightarrow (0.58 - 0.38)/(0.58 - 0.24) = 0.588$

For Unit 3 - Part D

- $1 - x_{LK3} = 1 - 0.44 = 0.56 = x_{HK3}$
- $1 - y_{LK3} = 1 - 0.78 = 0.22 = y_{HK3}$
- $OD = z_3 - y_{LK3} = 0.58 - 0.44 = 0.14$
- $DB = y_{LK3} - x_{LK3} = 0.78 - 0.44 = 0.34$
- $(OD/DB) \cdot F = V \quad (0.14/0.34) \cdot 0.58 = 0.239$
- $L = F - V = 0.58 - 0.239 = 0.341$
- $V^{\wedge}: V^{\wedge} = V/F = OD/DB = 0.14/0.34 = 0.412$
- $V: V = V^{\wedge} \cdot F = 0.412(40.72 \text{ kmol/hr}) = 16.78 \text{ kmol/hr} = V_3$
- $L = F - V = 40.72 - 16.78 = 23.94 \text{ kmol/hr} = L_3$

For Unit 4 - Part D

- $1 - x_{LK4} = 1 - 0.68 = 0.32 = x_{HK4}$
- $1 - y_{LK4} = 1 - 0.90 = 0.10 = y_{HK4}$
- $OD = z_4 - y_{LK4} = 0.78 - 0.68 = 0.10$
- $DB = y_{LK4} - x_{LK4} = 0.90 - 0.68 = 0.22$
- $(OD/DB) \cdot F = V \quad (0.10/0.22) \cdot 0.78 = 0.355$
- $L = F - V = 0.78 - 0.355 = 0.425$
- $V^{\wedge}: V^{\wedge} = V/F = OD/DB = 0.10/0.22 = 0.455$

- $V: V = V^*F = 0.455(16.78 \text{ kmol/hr}) = 7.62 \text{ kmol/hr} = V_4$
- $L = F - V = 16.78 - 7.62 = 9.16 \text{ kmol/hr} = L_4$

For Unit 5 - Part D

- $1 - x_{LK5} = 1 - 0.84 = 0.16 = x_{HK5}$
- $1 - y_{LK5} = 1 - 0.96 = 0.04 = y_{HK5}$
- $OD = z_5 - y_{LK5} = 0.90 - 0.84 = 0.06$
- $DB = y_{LK5} - x_{LK5} = 0.96 - 0.84 = 0.12$
- $(OD/DB)*F = V \quad (0.06/0.12)*0.90 = 0.45$
- $L = F - V = 0.90 - 0.45 = 0.45$
- $V^*: V^* = V/F = OD/DB = 0.06/0.12 = 0.50$
- $V: V = V^*F = 0.50(7.62 \text{ kmol/hr}) = 3.81 \text{ kmol/hr} = V_5$
- $L = F - V = 7.62 - 3.81 = 3.81 \text{ kmol/hr} = L_5$

rounding with good sense
0.948119 $\approx$ 0.95
(within calc. error.)

While it was predicted that five units were required to obtain a 95% purity of the light key in the vapor phase, we completed the project by obtaining a purity extremely close to that value. A great follow up to this design would be to optimize the process by manipulating temperature and pressure values using less equipment, creating a smaller and possibly more cost effective design.

Respectfully submitted,

Bryson Marshall
Zsamia Barnes

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
EQUILIBRIUM STAGED SEPARATION PROCESSES
SPRING 2021**

Instructor: Irvin W. Osborne-Lee

Title of Assignment

PROJECT 2 – *Graphical & Simulation Design of Distillation Column*

Outcome Measured Using this Assignment

Outcome 1

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

Check the complex engineering problem characteristics related to this assignment

Assignment problem	
	involves wide-ranging or conflicting technical issues,
X	has no obvious solution
	Addresses problems not encompassed by current standards and codes
	involves diverse groups of stakeholders
X	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
X	science
X	mathematics

Brief justification of why this assignment is suitable for this outcome

The design tasks lead to an open ended solution and involve an inter-related set of steps that require the student to employ math skills, knowledge of science including thermodynamics, and engineering concepts. Students must demonstrate understanding of phase equilibrium, ability to use material and energy balances, and skills with graphical methods and chemical process simulation.

Sample graded student's solution

Project 2
Team 3 Barnes
Franklin
Marshall

ABET EAC OUTCOME "1" RUBRIC

	(Excellent)	(Very Good)	(Average)	(Below Average)	(Poor)
Identify Formulate	1. Identify and Formulate engineering problems using principles of engineering/mathematics/science. Given a complex engineering problem (CEP), the student is able to: (i) Understand the given problem and identify the subject area and concepts involved. (ii) Convert the problem into a well labeled sketch. (iii) Formulate the CEP into a mathematical model stating all relevant assumptions. (iv) Formulate the CEP into an engineering model stating all relevant assumptions.	(i) Clearly identifies engineering problems beyond those discussed in class. Demonstrates very good understanding of the given problem and able to clearly identify the area and concepts involved. (ii) Consistently converts the problem into a well labeled sketch. Identifies the system of units applicable to the problem and uses them appropriately. (iii) Clearly defines the known and the unknown variables. (iv) States all relevant laws and equations. Lists and applies assumptions to the relevant laws and equations.	(i) Demonstrates adequate understanding of the given problem and reasonably able to identify the subject /topic area and concepts involved. (ii) In most cases converts the problem into a well labeled sketch. Fairly able to identify the system of units applicable to the problem and uses them most of the time. (iii) Adequately defines the known and the unknown variables. (iv) States most of the relevant laws and equations. Lists and applies most of the assumptions.	(i) Student unable to identify even those problems explicitly discussed in class. Does not show an understanding of the given problem and mostly unable to identify the area and concepts involved. (ii) Unable to convert the problem into a well labeled sketch. Rarely able to identify the system of units applicable to the problem and mostly does not show units. (iii) Poorly defines the known and the unknown variables. States very few of the relevant laws and equations needed. (iv) Unable to list and apply assumptions. Doesn't obtain specific solution to problem.	(i) Student unable to identify even those problems explicitly discussed in class. Does not show an understanding of the given problem and unable to identify the area and concepts involved. (ii) Unable to convert the problem into a well labeled sketch. Does not identify the system of units applicable to the problem and does not show units on work. (iii) Does not define the known and the unknown variables. Unable to state the relevant laws and equations. (iv) Unable to list/ apply assumptions. Unable to find the specific solution.
	Solve	2. Given a CEP that has been formulated, the student is able to: (i) Solve problem formulations using appropriate methods or tools. (ii) Evaluate and interpret the result.	(i) Implements very good strategy to solve the problem. Solves the problem and gets the right solution showing consistent units throughout. (ii) Evaluates and reasonably interprets the result.	(i) Implements strategy to solve the problem. Solves the problem and gets the right solution showing consistent units throughout. (ii) Evaluates and interprets the result.	(i) Implements fairly good strategy to solve the problem. Solves the problem and gets an acceptable solution mostly showing consistent units. (ii) Evaluates and provides a fair interpretation of the result.

100%

Excellent work!

Distillation Column Design Project

This assignment is a collaborative learning assignment. Work in teams self-assigned teams of three (use the People link in Canvas to join with teammates). Teams may consult each other but each team must prepare a project results poster presentation¹ in PowerPoint™ and submit a letter report² done up in Word™.

A binary mixture of components *A* and *B* is to be distilled in a continuous distillation tower operating at one atmosphere. The feed enters the column at a rate *F* in a saturated state (essentially at column pressure) with quality *χ* determined by the feed temperature *T_F*, and the feed composition *x_F* (the mole fraction of the light key in the feed). A distillate with purity *x_D* and a bottoms with composition *x_B* are to be achieved (for the light key) using a specified reflux ratio. See Table 1 for your team's particular design parameters. Complete the following tasks first using graphical methods, then with simulation.

- Determine the flow rates and compositions of the distillate and bottoms streams.
- Determine the number of theoretical trays needed if the column has a partial reboiler and a total condenser.
- Determine the minimum reflux ratio, *R_{min}* and the minimum boil-up ratio *V_{min}*.
- Determine the number of theoretical number of plates at minimum reflux, *N_M*.
- Determine the optimal feed location.
- For parts (a) through (e) above, compare your findings using the graphical methods with results from simulation using modeling software such as DWSIM (Short-Cut Column).
- Estimate the overall stage efficiency and actual number of trays, based on the given Murphree efficiency, then determine the height of your distillation tower.
- Estimate the flooding velocity and determine the diameter of your tower.
- Sketch your distillation tower showing the exterior dimensions, trays in their actual number, and annotate showing flow stream amounts, compositions, and state, plus energy stream amounts.
- As an alternative design, consider whether it would save energy if the reflux ratio is decreased to a value 20% above the minimum reflux ratio (ie. to $1.2R_{min}$). Compare the number of stages and energy consumption for the two alternatives.

VLE data can be obtained by literature search or by use of the DWSIM chemical process simulator. You must obtain the data for your *particular* system (see Table 1).

Team Members	Team	A	B	<i>F</i> Mol/s	<i>T_F</i> K	<i>x_F</i>	<i>R</i>	<i>x_D</i>	<i>x_B</i>	<i>E_M</i>
Irene, Ryan, Wasil	1	Toluene	M-xylene	300	403	0.33	2	0.95	0.05	0.45
Ebonie, Alexus, Cherish	2	P-xylene	O-ethyl toluene	250	427	0.44	2.3	0.97	0.07	0.50
Zsamia, Tyecia, Bryson	3	Toluene	Ethyl benzene	350	395	0.55	1.5	0.93	0.06	0.55
Cayla, Ike, Laura	4	Toluene	N-propyl benzene	400	400	0.66	1.7	0.98	0.04	0.60
Kibrom, Dayna Fredrick	5	Ethyl benzene	O-ethyl toluene	450	430	0.33	1.5	0.96	0.08	0.65
Michael	6	Ethyl benzene	O-diethyl benzene	300	440	.44	2.5	0.99	0.1	0.5

¹ The rubric showing the grading criteria for oral or video presentations is published at the eCourse site for this course.

² The format for the letter report is given in a sample report published at the eCourse site for this course.

Sunday, 4 April 2021

Bryson Marshall
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Dr. Osborne-Lee
CHEG 3043 Y01
VIA Canvas Upload

SUBJECT: Letter Report - Project 2 - Graphical & Simulation Design of Distillation Column

Dear Sir:

We are writing in regards to the course assignment posted to Canvas: *Upload letter report with Project 2 Findings*. The purpose of this report is to provide details on the design of a distillation tower using graphical and simulation methods. The given problem statement is displayed in Exhibit 1.

CHEG 3043 Equilibrium Staged Separation Processes <i>Graphical & Simulation Design of Distillation Column</i>	Project 2 <i>Tuesday 23 March 2021</i>
Flash and Flash Cascade Separation Design Project	
This assignment is a collaborative learning assignment. Work in teams self-assigned teams of three (use the People link in Canvas to join with teammates). Teams may consult each other but each team must prepare a project results poster presentation¹ in PowerPoint™ and submit a letter report² done up in Word™. A binary mixture of components <i>A</i> and <i>B</i> is to be distilled in a continuous distillation tower operating at one atmosphere. The feed enters the column at a rate <i>F</i> in a saturated state (essentially at column pressure) with quality <i>χ</i> determined by the feed temperature <i>T_F</i>, and the feed composition <i>x_F</i> (the mole fraction of the light key in the feed). A distillate with purity <i>x_D</i> and a bottoms with composition <i>x_B</i> are to be achieved (for the light key) using a specified reflux ratio. See Table 1 for your team's particular design parameters. Complete the following tasks first using graphical methods, then with simulation.	

Exhibit 1. This is the problem statement uploaded onto Canvas outlining the requirements and parameters for the design of the distillation column.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM, *Property Package Selection*. (last edited August 23, 2020). Last accessed February, 25, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

Along with the above problem statement in Exhibit 1, additional requirements were given, which are listed below.

- A. Determine the flow rates and compositions of the distillate and bottoms streams.
- B. Determine the number of theoretical trays needed if the column has a partial reboiler and a total condenser.
- C. Determine the minimum reflux ratio, R_{min} and the minimum boil-up ratio V_{min} .
- D. Determine the number of theoretical number of plates at minimum reflux, N_{Min} .
- E. Determine the optimal feed location.
- F. For parts (a) through (e) above, compare your findings using the graphical methods with results from simulation using modeling software such as DWSIM (Short-Cut Column).
- G. Estimate the overall stage efficiency and actual number of trays, based on the given Murphree efficiency, then determine the height of your distillation tower.
- H. Estimate the flooding velocity and determine the diameter of your tower.
- I. Sketch your distillation tower showing the exterior dimensions, trays in their actual number, and annotate showing flow stream amounts, compositions, and state, plus energy stream amounts.
- J. As an alternative design, consider whether it would save energy if the reflux ratio is decreased to a value 20% above the minimum reflux ratio (ie. to $1.2R_{min}$). Compare the number of stages and energy consumption for the two alternatives.

An often used separation process is one known as stage distillation or rectification. Our design specifically refers to a continuous distillation tower, in which the components to be separated are continuously fed to the tower. As a reference, *Transport Processes and Separation Process Principles* by C. J. Geankoplis, was used as guidance while completing the design project. In this process a distillation tower with multiple flash stages (also known as trays or sieve plates) allows for a liquid to flow down the column from one stage to the next, while the vapor bubbles upward from one stage to the one above¹. This creates a countercurrent flow through the vertically arranged trays and allows for the vapor and liquid to come in contact with one another¹. The two phases are in equilibrium as they exit the tray¹. The component with the lower boiling point is considered the more volatile component. As the more volatile component, which we consider the light key, moves upward from tray to tray, it becomes more concentrated in that particular compound.

The total condenser allows for the vapor product leaving the tower to be completely condensed back into liquid¹. The liquid is separated into two parts; the distillate and the reflux¹. The reflux flows back to the top tray of the tower¹. The reboiler, located near the bottom of the distillation tower, collects the liquid product¹. The reboiler, or partial reboiler in this case, allows for the product to be partially vaporized, collecting a product that has a high concentration of the less volatile component, or the heavy key¹. The vapor collected in the reboiler is returned to the

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM, *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

bottom tray of the tower¹. The product stream leaving the condenser is referred to as the distillate and the liquid stream leaving the reboiler is considered as the bottoms¹. The binary mixture, or feed, enters in the middle of the tower. The enriching section of the tower is located above the feed entrance, and is considered such due to the distillate being richer in the more volatile component¹. The enriching section also includes the total condenser¹. The stripping section is located below the feed entrance and includes the reboiler¹. Operating lines for the enriching section and stripping section aid in essential design steps such as the number of theoretical stages required through the use of the McCabe-Thiele method. These lines are usually drawn on a McCabe-Thiele diagram, an equilibrium curve diagram, along with a q-line using compositions and reflux ratios. Reflux ratio refers to the ratio of reflux and distillate separated from the condenser¹.

Methodology

Identify

An annotated sketch was performed on the distillation column displaying viable information that was provided with the problem statement. The feed stream is composed of toluene and ethylbenzene with a molar flow rate of 350 mol/s. The temperature of the feed, T_F , is 395 K. The feed composition, x_F , is 0.55 and represents the composition of the light key. Our light key was determined to be toluene due to its lower boiling point. Our heavy key was determined to be ethylbenzene. The composition of the light key in the distillate stream, x_D , is 0.93. The composition of the light key in the bottoms stream, x_B , is 0.06. Lastly, the provided reflux and Murphy efficiency given was 1.5 and 0.55, respectively. It is assumed that the liquid and vapor are in equilibrium before leaving a tray.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

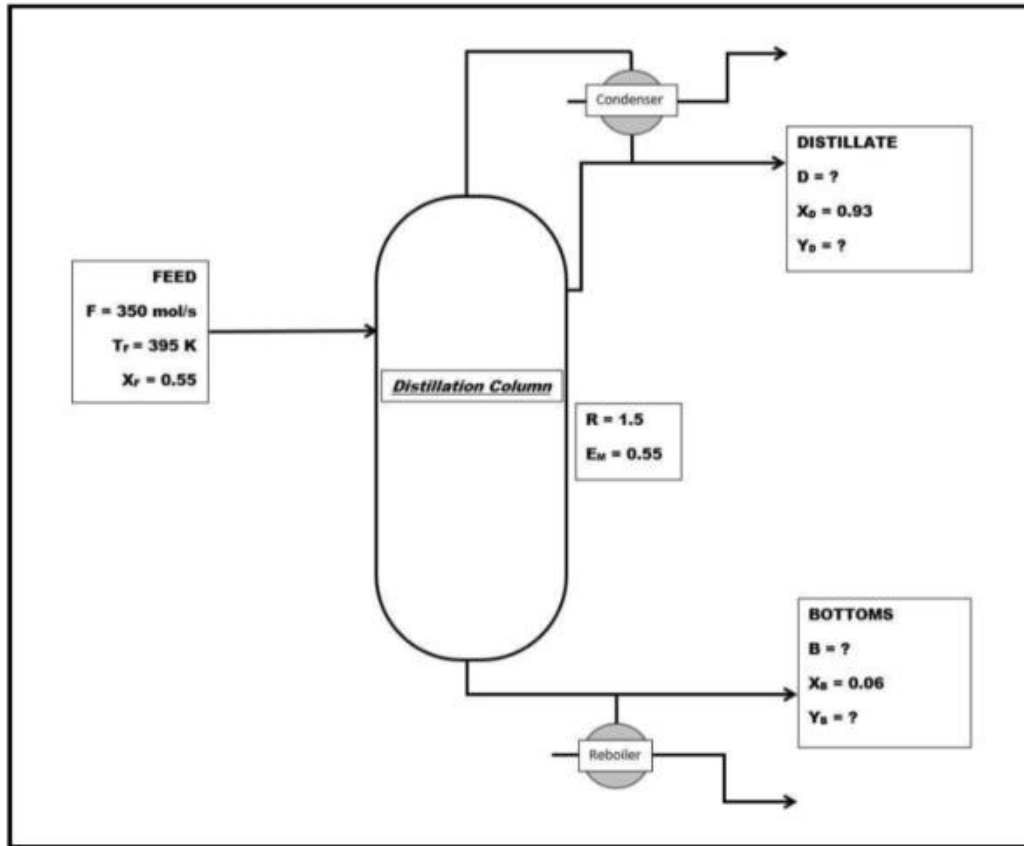


Figure 1. Annotated sketch used to identify the given information and the unknowns that remain to be determined.

Formulate

Several formulas were utilized in the design of the distillation column. These formulas are listed below.

Flow rates and compositions

$$F = D + B$$

$$F x_F = D x_D + B x_B$$

Enriching Operating Line

$$y = \frac{R}{R+1} x + \frac{x_D}{R+1}$$

Minimum Reflux Ratio, R_{min}

$$\frac{x_D - y'}{x_D - x'} = \frac{R_m}{R_m + 1}$$

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

Minimum Boilup Ratio, $V_{B, \min}$

$$V_{B, \min} = \frac{1}{(L/V) - 1}$$

Overall Tray Efficiency

$$E_o = \frac{\text{Number of theoretical trays}}{\text{Number of actual trays}}$$

$$E_o = \frac{\log[1 + E_M(mV/L - 1)]}{\log(mV/L)}$$

Height Equivalent To Theoretical Plate

$$HETP = \frac{T}{E_o}$$

Flow Factor Equation

$$\text{Flow Factor} = \frac{L}{V} \sqrt{\left(\frac{\rho_v}{\rho_L} \right)}$$

Flooding Velocity, U_c

$$U_c = K_V \sqrt{\frac{\rho_L - \rho_v}{\rho_v}} \left(\frac{\sigma}{20} \right)^{0.2}$$

Above Feed Stage

$$V = D(R + 1)$$

Below Feed Stage

$$V' = V_B B$$

Area of Column

$$A = \frac{\pi D^2}{4}$$

Analysis

Part A

An overall material balance was performed on the column and a material balance for toluene was then performed, as seen in Appendix: Calculations. The molar flow rate of the feed, the toluene compositions of the feed (x_F), distillate (x_D) and bottoms (x_B) were plugged into the material balance. This allowed for the molar flow rates of the distillate and bottoms molar flow rates to be determined. The remaining compositions of each stream were calculated by subtracting each given composition from one. The sum of all compositions for a given stream must equal one.

Part B

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

In order to determine the number of theoretical trays, a McCabe-Thiele diagram was created, as shown in Figure 2. First, an XY plot was generated using DWSIM modeling software. The Raoult's Law property package was selected for toluene and ethylbenzene based on their chemical properties and information in the package selection guide located in DWSIM². As seen previously in Figure 1, a Feed stream, Distillate product stream, and Bottoms product stream were selected and attached to a short-cut distillation unit. An energy stream for the total condenser and reboiler were also added. The given molar flow rate, temperature, and toluene compositions for each stream were applied to the unit. A short-cut distillation unit was utilized because valuable information such as the number of stages had not yet been determined. Once the simulation converged, an XY plot was able to be generated.

The problem statement mentioned that our feed stream was saturated. Knowing whether the feed stream is saturated liquid or vapor is required in order to determine the value of our q-line. The components in the binary mixture have boiling points below that of the feed temperature, which indicates our feed is saturated liquid. A saturated liquid results in a q line with a value of one; a vertical line extending from the feed composition¹. The q line serves at the intersection of the enriching operating line and stripping operating line. The slope of the enriching operating line was calculated using the formula listed previously. The slope of 0.60 was plotted on the McCabe-Thiele diagram using the coordinates (0.93, 0.92) as a reference point. This is where the composition, x_D , intersects the 45° line. To confirm the proper placement of the enriching line, a line was drawn from a point on the 45° line, using x_D , to the q line. From the q line, a line was drawn to point the point x_B . This line represents the stripping operating line. The intersection represents a pinch point; the lines intersect on the q-line and equilibrium line.

To determine the theoretical trays, the step down method is used. Starting at x_D , a step down is drawn from the enriching line to the equilibrium line and then from the stripping line to the equilibrium after passing the q line. The composition, x_B , is used as the stopping point. There are 18 theoretical steps resulting in 16 theoretical stages plus one stage for the total condenser and one for the partial reboiler.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

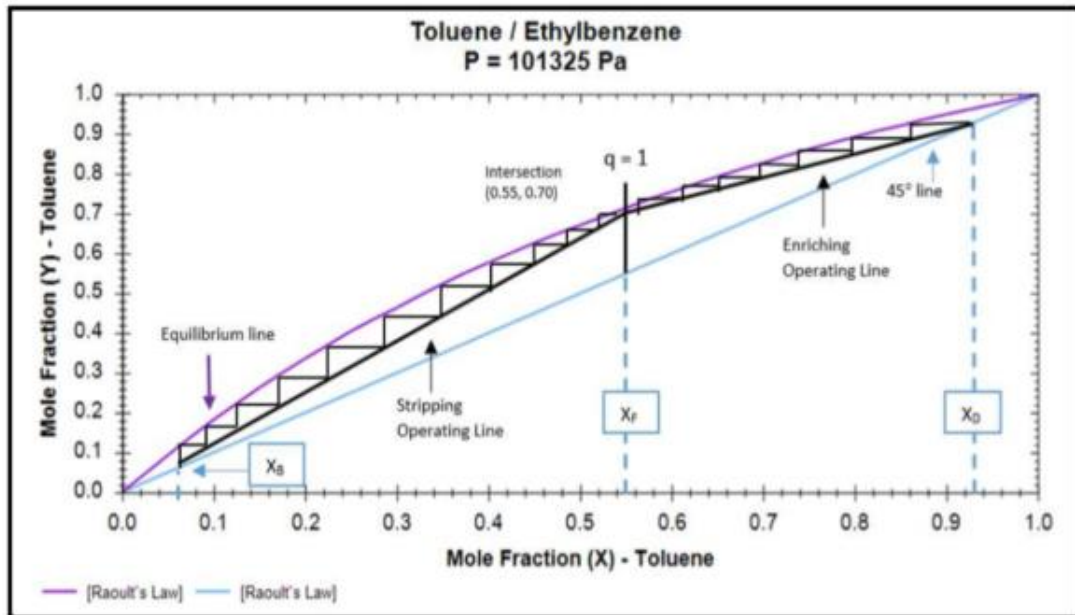


Figure 2. McCabe-Thiele diagram for toluene and ethylbenzene using an XY diagram generated by DWSIM. The diagram displays the number of theoretical stages using the enriching and stripping operating lines.

Part C

Part C involved the calculations of the minimum reflux ratio and minimum boilup ratio, which can be found in Appendix: Calculations. The minimum reflux ratio, R_{min} , is the smallest value that allows for an infinite number of stages in order to achieve the desired separation¹. The pinch point, displayed in Figure 2, is a result of a decrease in reflux ratio, as well as in the slope of the enriching operating line¹. The value, $R_{min} = 1.37$, was found using the equation provided in the Formulas section. A reflux of at least 1.37, must be used in order to achieve the desired purity.

The minimum boilup ratio, $V_{B,min}$, is the minimum ratio required for desired separation. It is the minimum ratio of liquid being returned to the tower to the liquid leaving in the bottoms stream. In order to perform the calculation, it was important to consider the conditions of the feed stream. The feed stream enters as saturated liquid or bubble-point liquid, indicating the conditions to find $\bar{L}$ and $\bar{V}$. Our vapor stream remains unaffected by the temperature of the feed, so $\bar{V} = V$. The minimum boilup ratio of 0.64 was found using the equation in the formula section.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM, *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

Part D

To determine the number of theoretical plates at minimum reflux, N_{min} , we used the McCabe Thiele method. Starting at the X_D location drawing a horizontal line from the bubble curve to the dew curve, then drawing a vertical line from the dew curve to the bubble curve. We continued to do this method until we passed the X_B location. From using the method previously explained we found that the theoretical number of plates at minimum reflux, N_{min} , would be 8 plates. The number of theoretical plates can be seen in Figure 3.

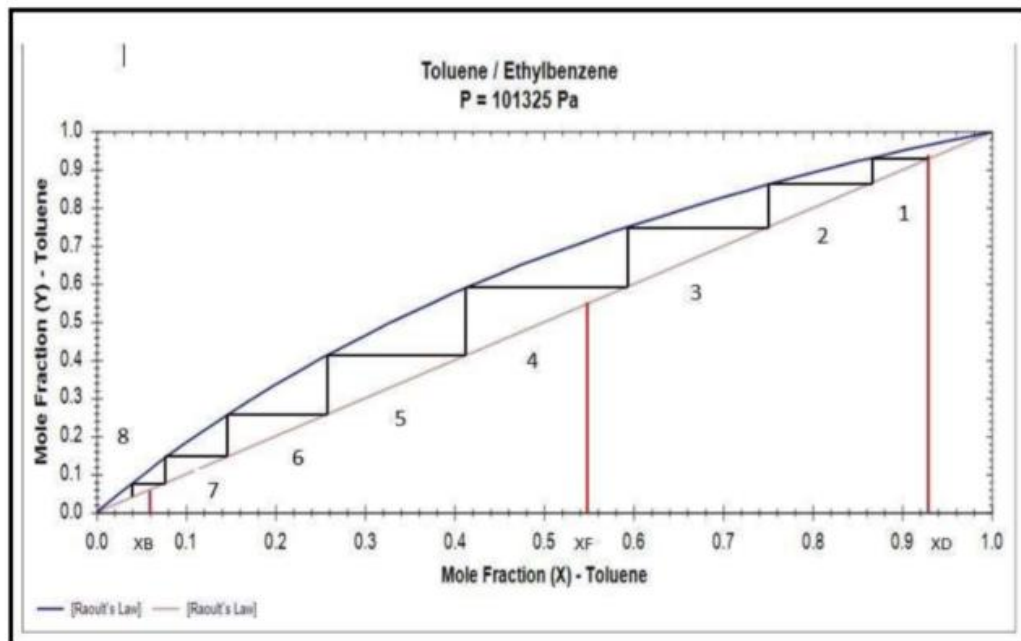


Figure 3. XY Diagram using McCabe Thiele method to show number of theoretical plates

Part E

To determine the optimal feed location, the McCabe Thiele step-down method was used. Starting at the X_D , a line was drawn from the enriching operating line to the equilibrium curve, continuing past the q-line. This continues from the stripping operating line until reaching the X_B location. The optimal feed location will be where the q-line passes through a stage, as shown in

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

Figure 4. The q-line line passes through the 8th tray and that is the most optimal location for the feed.

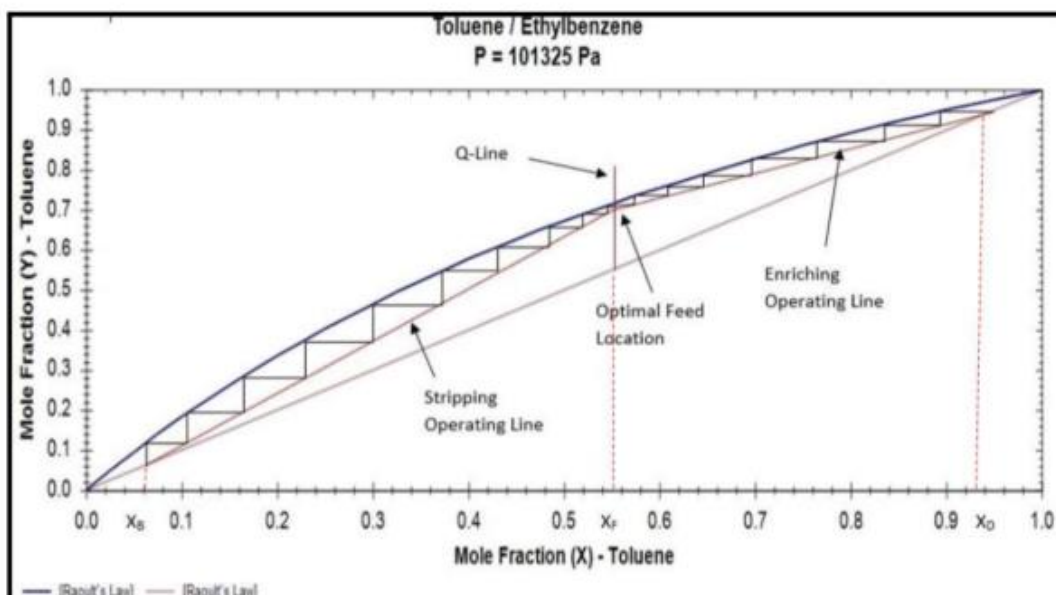


Figure 4. XY plot of Toluene and Ethylbenzene, showing the optimal feed location.

Part F

In order to compare findings on Part F for Parts A-E, we used the DWSIM modeling software results to compare our graphical methods to theoretically determine how many plates were needed for the column. A Short-Cut Column was designed in order to display and compare the findings. For part A, we needed to determine the flow rates and compositions of the distillate and bottoms streams. From the calculations, the distillate has a flow rate of 197.126 mol/s and the bottoms has a flow rate of 152.873 mol/s. Compared to the simulation results the distillate has a flow rate of 205.434 mol/s and the bottoms has a flow rate of 144.572 mol/s. Next, comparison for part B was the number of theoretical trays needed with a partial reboiler and condenser. Using the McCabe Theile graphical method it was found that there are 18 trays needed, while from the simulation it was discovered that there are 19 trays needed. This shows that it was relatively close with the number of theoretical trays needed. For part C, it was found that the reflux ratio from DWSIM is 1.68, and from the calculations our reflux ratio is 1.37. From the simulations increase of the reflux ratio it will raise the purity of the distillate. As well for part D the McCabe-Theile method was used to determine the theoretical number of trays at minimum reflux. From the graphical method we found that the minimum number of trays needed was 8 trays, while from the simulation we found that the distillation tower needed a minimum of 10

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

trays. Finally, part E we determined that the optimal feed location using the McCabe-Theile method was at the 8th tray. From DWSIM it shows that the optimal feed location is at the 13th tray, in all probability this is due to us not having the same number of trays from the graphical method compared to the simulation.

Part G

Part G used different calculations to determine the overall stage efficiency, the actual number of trays, and to determine the height of the distillation tower. First, we found the overall stage efficiency by using the equation $E_o = \frac{\log[1+E_M(mV/L-1)]}{\log(mV/L)} E_M$, was the given Murphree tray efficiency which was 0.55. The slope of the equilibrium line in the equation is represented by m . L/V in the equation is the inverse of the slope of the Enriching operating line. After our calculations we found that the overall efficiency was 0.686.

Then we went on to find the actual number of trays needed, which was found by the equation $E_o = \frac{\text{Number of theoretical trays}}{\text{Number of actual trays}}$. E_o , which is the overall tray efficiency was previously found to be 0.686. The number of theoretical trays without the condenser and partial reboiler is 16 trays. We then divided the number of theoretical trays by the overall tray efficiency to find the number of actual trays, which came out to be 23.3 actual trays.

Then to determine the height of the distillation tower, we first used the equation, $HETP = \frac{T}{E_o}$.

T , is found to be the tray spacing, for our distillation tower the tray spacing will be 450 mm. The calculated number of HETP is 653.35. Finally, to find the actual height of the distillation tower we used $H = n(HETP)$, n represents the number of theoretical stages. From the calculations our height of the distillation tower is 11.76 meters(11760.2 mm).

Part H

The first segment of Part H consisted of estimating the flooding velocity of the distillation column. Before solving the flooding velocity U_c equation, we needed to determine the Flow Factor which involved using the ratio of the mass flowrate of the liquid (L) to vapor (V) that was solved for in *Part A* and the density of each phase that was given in our thermodynamic model simulation results displayed in Figure 5. The flow factor turned out to be 0.050. Next, we used the flow factor and size of the tray spacing within the column to assist with determining our K_v value. The K_v value is a constant used for the flooding velocity U_c equation. In order to find K_v we used a graph in the course textbook for the estimation of K_v value for allowable vapor velocity shown below in Figure 6¹. Using the graph, we started at our flow factor of 0.050 on the x-axis($F_{lv} = \frac{L}{G} (\frac{\rho_g}{\rho_l})^{0.5}$) and drew a red line vertically until it touches the "plate spacing"

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM, *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

line for 18 inches since our actual tray spacing is 17.7 inches. Once we reached the “plate spacing” line we then drew a perpendicular line to the y-axis(

$$C_{sb, flood} = U_{nf} \left(\frac{20}{\sigma} \right)^{0.2} \left(\frac{\rho_l}{\rho_l - \rho_g} \right)^{0.5}, \text{ft/s) from that point to determine the } K_v \text{ value of 2.80.}$$

Property	Value	Units
Volumetric Flow Rate @ T, P	0.0242237	m ³ /s
Mass Flow Rate	18.4379	kg/s
Molar Flow Rate	173.9	mol/s
Phase Molar Fraction	0.993715	
Phase Mass Fraction	0.993723	
Compressibility Factor	0	
Specific Enthalpy	-178.408	kJ/kg
Molar Enthalpy	-18915.9	kJ/kmol
Specific Entropy	-0.370842	kJ/(kg·K)
Molar Entropy	-39.3187	kJ/(kmol·K)
Internal Energy	-178.408	kJ/kg
Molar Internal Energy	-18915.9	kJ/kmol
Gibbs Free Energy	-26.7601	kJ/kg
Molar Gibbs Free Energy	-2837.26	kJ/kmol
Helmholtz Free Energy	-26.7601	kJ/kg
Molar Helmholtz Free Energy	-2837.26	kJ/kmol
Molecular Weight	106.026	kg/kmol
Density	761.149	kg/m ³
Heat Capacity (Cp)	2.13503	kJ/(kg·K)
Heat Capacity Ratio (Cp/Cv)	1	
Thermal Conductivity	0.103553	W/(m·K)
Kinematic Viscosity	3.26134E-07	m ² /s
Dynamic Viscosity	0.000245201	Pa·s
Surface Tension	0.018819	N/m

Property	Value	Units
Volumetric Flow Rate @ T, P	0.0249034	m ³ /s
Thermal Conductivity	0.0199929	W/(m·K)
Speed of Sound	183.655	m/s
Specific Enthalpy	0.454422	kJ/(kg·K)
Specific Entropy	157.597	kJ/kg
Phase Molar Fraction	0.00629472	
Phase Mass Fraction	0.0062766	
Molecular Weight	105.888	kg/kmol
Molar Internal Energy	-3.38316E+06	kJ/kmol
Molar Helmholtz Free Energy	-3.45283E+06	kJ/kmol
Molar Gibbs Free Energy	-2989.16	kJ/kmol
Molar Flow Rate	1.09993	mol/s
Molar Entropy	48.1177	kJ/(kmol·K)
Molar Enthalpy	16687.6	kJ/kmol
Mass Flow Rate	0.116458	kg/s
Kinematic Viscosity	3.00349E-06	m ² /s
Joule Thomson Coefficient	4.69583E-08	K/Pa
Isothermal Compressibility	9.86523E-06	1/Pa
Internal Energy	-31950.4	kJ/kg
Helmholtz Free Energy	-32136.2	kJ/kg
Heat Capacity Ratio (Cp/Cv)	1.05049	
Heat Capacity (Cp)	1.63366	kJ/(kg·K)
Gibbs Free Energy	-28.2295	kJ/kg
Dynamic Viscosity	9.47827E-06	Pa·s
Density	3.15576	kg/m ³
Compressibility Factor	1	

Figure 5. The Overall Liquid(left) and Vapor(right) Thermodynamic Simulation Model Phase Property Results generated from the DWSIM software for Toluene and Ethylbenzene ²

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed, (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforinside.com.br/wiki/index.php?title=Property_Package_Selection

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

Team 3, Project 2

Page 12

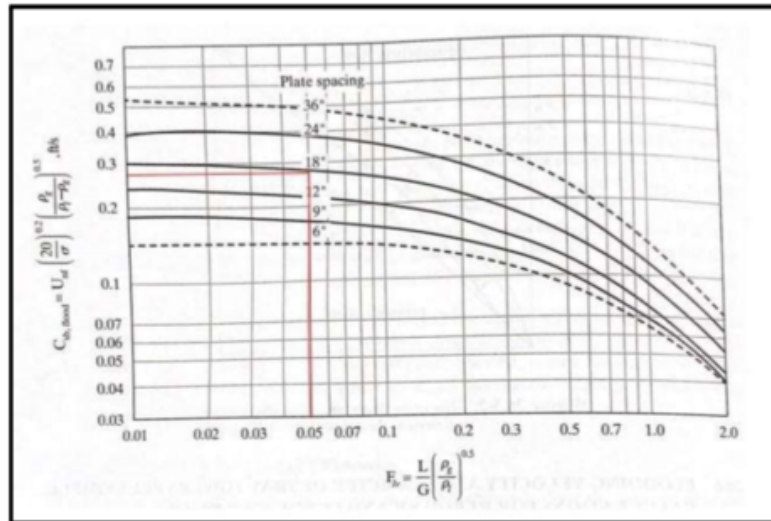


Figure 6. Estimation of Kv values for allowable vapor velocity. From Fair, J. R., *Petro/Chem. Eng.*,33(10) 45 (1961) graph given in the textbook on page 840 ¹

When proceeding to calculate the flooding velocity U_c values were able to be plugged in the equation because they were either given them in our thermodynamic model simulation or have previously solved them. The surface tension, vapor density, and liquid density are all given in the simulation results displayed in Figure 5². The flooding velocity U_c equation identifies the maximum permissible vapor velocity for the column. Using the equation found in the *Formula* section we were able to find the flooding velocity of the distillation column design to be 12.82m/s.

The next segment of Part H involves determining the diameter of the tower. Before we determined the diameter of the distillation column the volumetric flow rate for the reboiler and feed stage. In order to complete the calculations the above feed stage and below feed stage had to be calculated using the equations in the *Formulas* section prior. The calculations for the Above Stage Feed is 492.82 mol/s and the Below Stage Feed is 99.37 mol/s. Next, we began to find the temperatures of the reboiler stage and the feed stage by using the T-xy diagram above in Figure 7 by drawing a vertical line from the x-axis (mole fractions) until it reaches the dew point line (aqua line) and a perpendicular horizontal line to the y-axis (temperature). The reboiler stage temperature is 408.5 K. The feed stage temperature is 398 K. At 408.5 K the volumetric flow rate for the reboiler was 3.32 m³/s and at 398 K the volumetric flow rate for the feed stage was 16.10 m³/s. Since we wanted to design our column based on the highest flow rate possible we used the volumetric flow rate for the feed stage. Then we divided our feed stage volumetric flow rate by the flood velocity, 12.82m/s so it would agree with the Area formula. The final step was

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

to determine the diameter of the distillation tower by using the Area formula given in the Formulas section to solve for D (diameter). The diameter of the distillation tower was 1.60 m.

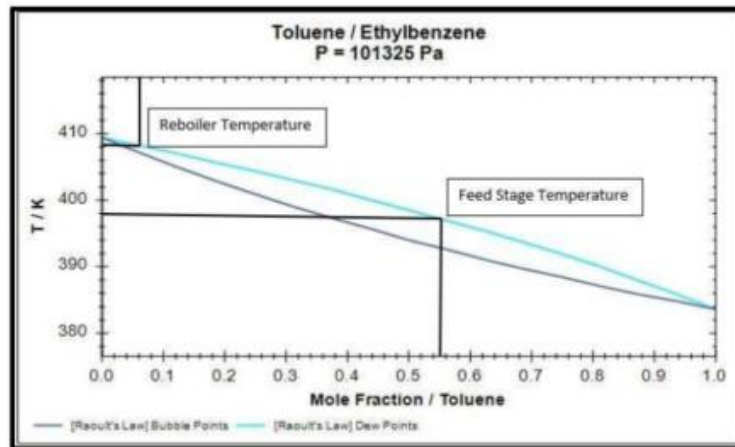


Figure 7. T-xy diagram for Toluene generated by DWSIM displaying the temperatures for the specific mole fractions for the Reboiler Stage and Feed Stage ²

Part I

After completing all required calculations, a sketch was made to better illustrate the design parameters of the distillation tower as seen below in Figure 8.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM, *Property Package Selection*, (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

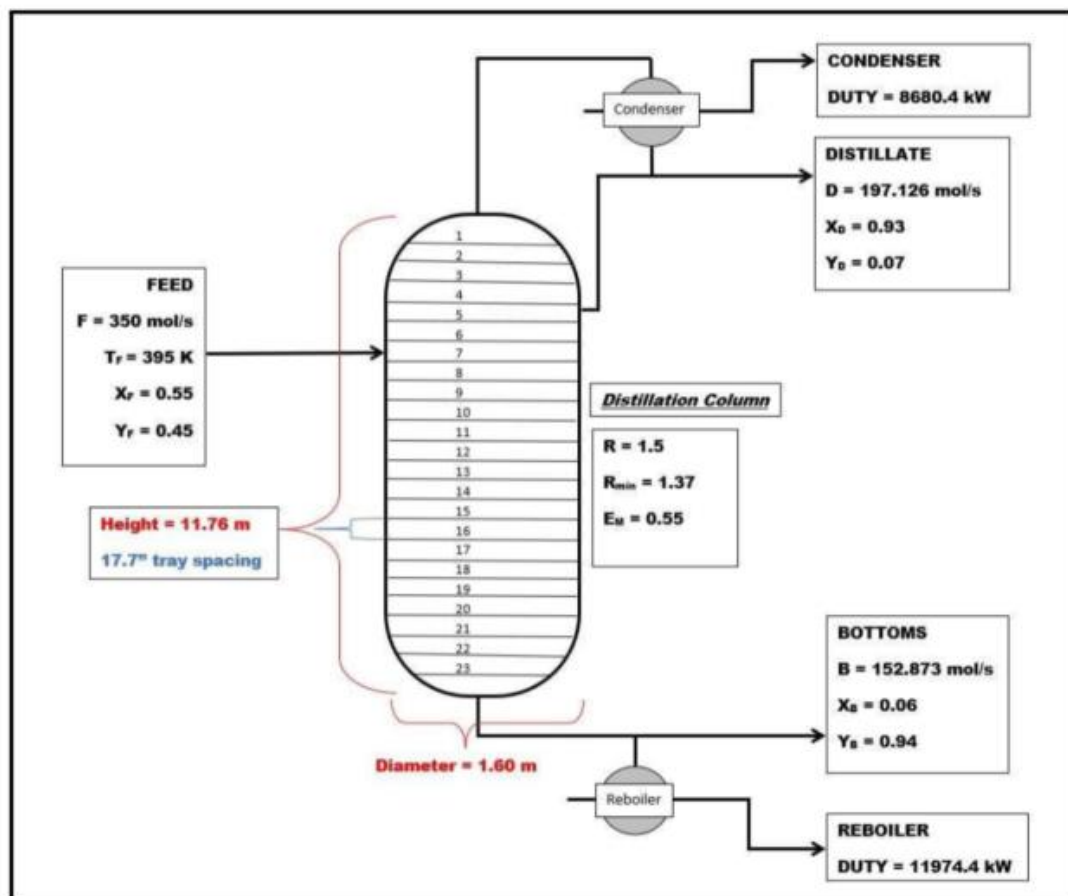


Figure 8. Sketch of the Distillation Column showing exterior dimensions, actual number of trays, and annotations displaying flow stream amounts, compositions, state, and the energy streams

Part J

Part J incorporated us creating an alternative design to compare results to our original design results if we adjusted the reflux ratio. The reflux ratio was changed to a value 20% above the minimum reflux ratio R_{min} . Using the original reflux ratio of 1.5 given, we obtained the results displayed in Figure 9: condenser duty 8680.4 kW and the reboiler duty of 11974.4 kW². The new reflux ratio for this design was 1.64. Having a reflux ratio of 1.64 gave us the results shown below in Figure 10: condenser duty: 9490.57 and the reboiler duty of 12784.6 kW. Comparing

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforinside.com.br/wiki/index.php?title=Property_Package_Selection

these results the alternative design did not help us save energy due to the increase in the utility duties, yet the number of stages remained the same.

Property	Value	Units
Minimum Reflux Ratio	2.0225	
Minimum Number of Stages	12.8448	
Actual Number of Stages	NaN	
Optimal Feed Stage	NaN	
Stripping Liquid	532.829	mol/s
Rectify Liquid	262.5	mol/s
Stripping Vapor	357.829	mol/s
Rectify Vapor	437.5	mol/s
Condenser Duty	8680.4	kW
Reboiler Duty	11974.4	kW

Figure 9. Condenser and Reboiler Duty from the Thermodynamic Simulation Model Phase Property Results generated from the DWSIM software for Toluene and Ethylbenzene ²

Property	Value	Units
Minimum Reflux Ratio	2.0225	
Minimum Number of Stages	12.8448	
Actual Number of Stages	NaN	
Optimal Feed Stage	NaN	
Stripping Liquid	557.329	mol/s
Rectify Liquid	287	mol/s
Stripping Vapor	382.329	mol/s
Rectify Vapor	462	mol/s
Condenser Duty	9490.57	kW
Reboiler Duty	12784.6	kW

Figure 10. Condenser and Reboiler Duty from the Thermodynamic Simulation Model Phase Property Results for the alternative design generated from the DWSIM software for Toluene and Ethylbenzene ²

All requirements were completed for this assignment. This project has demonstrated that more trays leads to higher purity for separation, however cost analysis would be a great follow-up project. Manipulating design parameters such as reflux ratio or adding additional trays would affect cost, but it would be interesting to know by how much.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

Respectfully submitted,

Bryson Marshall

Tyecia Franklin

Zsamia Barnes

would be helpful to
show your simulated
flowsheet.

Appendix: Calculations

The following calculations were used in the design of the project.

Part A

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

- $Fx_F = Dx_D + Bx_B \rightarrow 350 \text{ mol/s} (0.55) = 0.93D + 0.06B$
- $192.5 = 0.93D + 0.06B \rightarrow 192.5 = 0.93D + 0.06(350-D)$
- $192.5 = 0.87D + 21 \rightarrow 171.5 = 0.87D \rightarrow D = 197.126 \text{ mol/s}$
- $F = D + B \rightarrow B = 350 - 197.126 \rightarrow B = 152.873 \text{ mol/s}$
- $1 - x_F = 1 - 0.55 = 0.45 \text{ heavy key in feed}$
- $1 - x_D = 1 - 0.93 = 0.07 \text{ heavy key in distillate}$
- $1 - x_B = 1 - 0.06 = 0.94 \text{ heavy key in bottoms}$

Part B

- $y = \frac{R}{R+1}x + \frac{x_D}{R+1} \rightarrow y = \frac{1.5}{1.5+1}x + \frac{0.93}{1.5+1} \rightarrow y = 0.60x + 0.372$
- Slope of enriching line: **0.60**

Part C

- $\frac{x_D - y'}{x_D - x'} = \frac{Rm}{Rm + 1} \rightarrow \frac{0.93 - 0.71}{0.93 - 0.55} = \frac{Rm}{Rm + 1}$
- $0.5789 = \frac{Rm}{Rm + 1}$
- Let $R_m = x \rightarrow 0.5789 = \frac{x}{x + 1}$
- $x = 0.5789x + 0.5789$
- $0.4211x = 0.5789 \rightarrow x = 1.37 = R_{\min}$
- For bubble point liquid feed, $\bar{L} = L + V$ and $V = \bar{V}$
- $\bar{L} = (152.873 + 350) \text{ mol/s} = 502.837 \text{ mol/s}$
- $V = 197.126 \text{ mol/s}$
- $V_{B,MIN} = \frac{1}{(L/V) - 1} = \frac{1}{(502.837/197.126) - 1} = 0.65 = V_{B,MIN}$

Part G

- Overall tray efficiency $= E_o = \frac{\log[1 + E_M(mV/L - 1)]}{\log(mV/L)}$
- $E_o = \frac{\log[1 + 0.55(2.5/3 - 1)]}{\log(2.5/3)} = 0.686$
- $E_o = \frac{\text{Number of theoretical trays}}{\text{Number of actual trays}}$
- Number of actual trays $= \frac{16}{0.686} = 23.3$ actual trays
- $HETP = \frac{T}{E_o} = \frac{450}{0.686} = 653.35$
- $H = n(HETP) = 18(653.35) = 11760.2 \text{ mm} = 11.76 \text{ meters}$

Part H

- Flow Factor $= \frac{L}{V} \sqrt{\left(\frac{\rho_v}{\rho_l}\right)}$
- $L/V = \text{Ratio of mass flow rate of Liquid to Vapor}$
- $\frac{152.87}{197.126} \sqrt{\left(\frac{3.15 \text{ kg/m}^3}{761.15 \text{ kg/m}^3}\right)} = 0.050$

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² DWSIM. *Property Package Selection*. (last edited August 23, 2020). Last accessed March 30, 2021 at https://dwsim.inforside.com.br/wiki/index.php?title=Property_Package_Selection

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
EQUILIBRIUM STAGED SEPARATION PROCESSES
SPRING 2021**

Instructor: Irvin W. Osborne-Lee

Title of Assignment

PROJECT 3 – *Design of Liquid-Liquid Extraction System and
Comparison of Alternatives*

Outcome Measured Using this Assignment

Outcome 1

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

Check the complex engineering problem characteristics related to this assignment

Assignment problem	
	involves wide-ranging or conflicting technical issues,
X	has no obvious solution
	Addresses problems not encompassed by current standards and codes
	involves diverse groups of stakeholders
X	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
X	science
X	mathematics

Brief justification of why this assignment is suitable for this outcome

The design tasks lead to an open ended solution and involve an inter-related set of steps that require the student to employ math skills, knowledge of science including thermodynamics, and engineering concepts. Students must demonstrate understanding of phase equilibrium, ability to use material and energy balances, and skills with graphical methods and comparison of alternative cascade configurations.

Sample graded student team's solution

Team 3
Barnes & Marshall

ABET EAC OUTCOME "1" RUBRIC

	(Excellent)	(Very Good)	(Average)	(Below Average)	(Poor)
1. Identify and Formulate engineering problems using principles of engineering/mathematics/science. Given a complex engineering problem (CEP), the student is able to:	(i) Clearly identifies engineering problems beyond those discussed in class. Demonstrates very good understanding of the given problem and able to clearly identify the area and concepts involved.	(i) Demonstrates understanding of the given problem and able to identify the area and concepts involved.	(i) Demonstrates adequate understanding of the given problem and reasonably able to identify the subject /topic area and concepts involved.	(i) Student unable to identify even those problems explicitly discussed in class. Does not show an understanding of the given problem and mostly unable to identify the area and concepts involved.	(i) Student unable to identify even those problems explicitly discussed in class. Does not show an understanding of the given problem and unable to identify the area and concepts involved.
(ii) Understand the given problem and identify the subject area and concepts involved.	(ii) Consistently converts the problem into a well labeled sketch. Identifies the system of units applicable to the problem and uses them appropriately.	(ii) Converts the problem into a well labeled sketch. Identifies the system of units applicable to the problem and uses them appropriately.	(ii) In most cases converts the problem into a well labeled sketch. Fairly able to identify the system of units applicable to the problem and uses them most of the time.	(ii) Unable to convert the problem into a well labeled sketch. Rarely able to identify the system of units applicable to the problem and mostly does not show units.	(ii) Unable to convert the problem into a well labeled sketch. Does not identify the system of units applicable to the problem and does not show units on work.
(iii) Formulate the CEP into a mathematical model stating all relevant assumptions.	(iii) Clearly defines the known and the unknown variables.	(iii) Defines the known and the unknown variables.	(iii) Adequately defines the known and the unknown variables.	(iii) Poorly defines the known and the unknown variables.	(iii) Does not define the known and the unknown variables.
(iv) Formulate the CEP into an engineering model stating all relevant assumptions.	(iv) States all relevant laws and equations. Lists and applies assumptions to the relevant laws and equations.	(iv) States relevant laws and equations. Lists and applies assumptions to the relevant laws and equations.	(iv) States most of the relevant laws and equations. Lists and applies most of the assumptions.	(iv) States very few of the relevant laws and equations needed.	(iv) Unable to state the relevant laws and equations.
2. Given a CEP that has been formulated, the student is able to:	(i) Implements very good strategy to solve the problem. Solves the problem and gets the right solution showing consistent units throughout.	(i) Implements strategy to solve the problem. Solves the problem and gets the right solution showing consistent units throughout.	(i) Implements fairly good strategy to solve the problem. Solves the problem and gets an acceptable solution mostly showing consistent units.	(i) Implements poor strategy to solve the problem. Unable to solve the problem and usually gets the wrong solution. Does not show consistent units, mostly.	(i) Implements poor strategy to solve the problem. Unable to solve the problem and usually gets the wrong solution. Does not show consistent units.
(ii) Evaluate and interpret the result.	(ii) Evaluates and reasonably interprets the result.	(ii) Evaluates and interprets the result.	(ii) Evaluates and provides a fair interpretation of the result.	(ii) Seldom evaluates and provides an interpretation of result.	(ii) Does not evaluate and nor interpret the result.

98%

Design of Liquid-Liquid Extraction System and Comparison of Alternatives

This assignment is a collaborative learning assignment. Work in teams self-assigned teams of two as assigned. Teams may consult each other but each team must prepare a project results poster presentation¹ in PowerPoint™ and submit a letter report² done up in Word™.

You will do your analysis for a ternary system consisting of a carrier and solute, plus a solvent. Each team will work with a different ternary system, which will be found by literature search and consultation with instructors, who can direct the student to possible sources for ternary system LLE data.

Your team will complete its design by constructing a ternary diagram with LLE data plotted for your particular (approved) ternary system. Use the feed stream flow rate F and composition x_B^F assigned in the table below. Also, use the solvent composition x_C^S assigned in the table below, assuming no carrier enters in the solvent stream.

Consider three design alternatives, as listed below.

- A single stage LLX.
- Counter-current cascade, with the fresh feed stream entering the first unit and the fresh solvent stream entering the last unit; and the product extract stream leaving the first unit and the product raffinate stream leaving the last unit. In this cascade mode, determine the number of stages needed to achieve the assigned product composition, x_B^F .
- Cross-current cascade having the same number of units as that in alternative (b) above, with the raffinate from each unit used as the feed stream for the next unit (except the last, of course); the extract stream leaving each unit combining into a single product stream; and the solvent stream entering each unit in an amount equal to the solvent stream amount in (b) above divided by the number of units. In this cascade mode, determine the final product purity x_B^F .
- Discuss the performance of each LLX operational alternative. What are the advantages and disadvantages (if any) of each mode of operation?

LLE data must be obtained by literature search. You may select your team's *particular* system (or it will default to that designated in Table 1) – this may be accomplished in the initial consultation for your team for this project.

	Team	Ternary Mixture Components			T, K	$F, \text{kmol/hr}$	x_B^F	x_C^S	x_B^F
1	Alexander & Livingston	Water	Butyric Acid	Diethyl Succinate	298	1,250	0.10	0.96	0.80
2	Anaghara & Lovelace	Water	Butyric Acid	Diethyl Glutarate	298	1,000	0.15	0.97	0.60
3	Atatah & Mahmood	Water	Butyric Acid	Diethyl Adipate	298	750	0.20	0.98	0.65
4	Barnes & Marshall	Water	Morpholine	Dimethyl Phthalate	298	500	0.10	0.99	0.50
5	Chioma Nkemadu	Water	Morpholine	Ethyl Nonaoate	298	1,250	0.15	0.99	0.70
6	Franklin & Ukpede	Water	Morpholine	Isoamyl Alcohol	298	1,000	0.20	0.98	0.55
7	Henderson & Vaughn	Water	Propionic Acid	Diethyl Succinate	298	500	0.15	0.96	0.40
8	Asfaha, Butler, Williams	Water	Butyric Acid	Oleyl Alcohol	298, 318	750	0.10	0.97	0.60

¹ The rubric showing the grading criteria for oral or video presentations is published at the eCourse site for this course.

² The format for the letter report is given in a sample report published at the eCourse site for this course.

Bryson Marshall
Zsamia Barnes
Students, CHEG 3043 Y01
VIA email:
bmarshall11@pvamu.edu
zbarnes3@pvamu.edu

Dr. Osborne-Lee
CHEG 3043 Y01
VIA Canvas Upload

SUBJECT: Letter Report - Project 3: Design of Liquid-Liquid Extraction System and Comparison of Alternatives

Dear Sir:

I am writing in regards to the course assignment posted to Canvas: *Upload letter report with Project 3 Findings*. The assignment requires a ternary system to be constructed by plotting liquid-liquid extraction (LLX) data given in the problem statement. The three design alternatives below, along with their requirements, are required to be constructed and analyzed.

- A single stage LLX
- Counter-current cascade, with the fresh feed stream entering the first unit and the fresh solvent stream entering the last unit; and the product extract stream leaving the first unit and the product raffinate stream leaving the last unit. In this cascade mode, determine the number of stages needed to achieve the assigned product composition, x_B^E .
- Cross-current cascade having the same number of units as that in alternative (b) above, with the raffinate from each unit used as the feed stream for the next unit (except the last, of course); the extract stream leaving each unit combining into a single product stream; and the solvent stream entering each unit in an amount equal to the solvent stream amount in (b) above divided by the number of units. In this cascade mode, determine the final product purity x_B^E .
- Discuss the performance of each LLX operational alternative. What are the advantages and disadvantages (if any) of each mode of operation?

Liquid-liquid extraction is a separation process that involves the separation of compounds based on the physical and chemical properties¹. The process typically includes three components: the extract, the carrier and the solvent. For the single stage LLX, two separate streams enter the separation unit; one containing the solute and carrier components, known as the feed stream, and the solvent stream. For this project, we assume that no solvent enters the feed stream, however this is a possibility. The two product streams that exit the unit are known as the raffinate and extract streams. The extract stream is considered as the solvent-rich product stream. The raffinate

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/jc1000022>.

stream is considered the carrier-rich product stream. This depends on the carrier being immiscible or partially soluble within the solvent ¹.

The three types of liquid-liquid extraction techniques discussed include single stage equilibrium extraction, countercurrent extraction, and crosscurrent extraction. Single stage involves the transfer of the solute between the two liquids when the phases come in contact with one another. Countercurrent and crosscurrent extraction are multistage techniques. In countercurrent extraction, the feed and solvent streams enter the system at opposite ends while the raffinate and extract product streams flow countercurrently ¹. In crosscurrent extraction, the feed streams enter the first stage from the top of the first stage while a fresh solvent stream enters the side of each stage ¹.

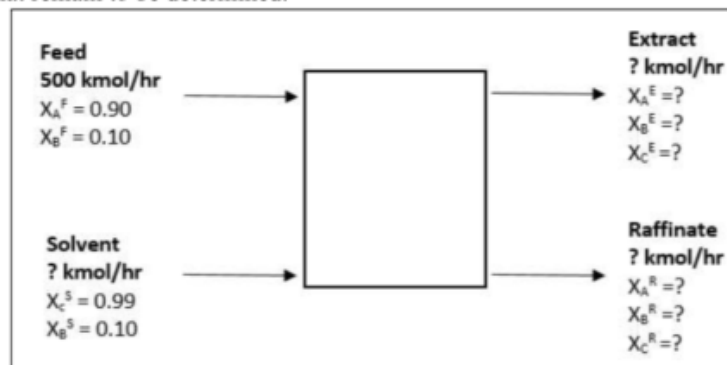
For this design, a ternary diagram displaying equilibrium data for a three-component system is used. The area under the phase curve, known as the equilibrium line, represents two phases in which the compositions at equilibrium can be determined ¹.

Methodology

Identify

A single stage LLX, as seen below in Figure 1, was labeled with the molar flow rate for the feed and compositions given in the problem statement. The three components given include dimethyl phthalate (component A), morpholine (component B), and water (component C). With guidance from a literature review of work performed by Lutfullah M. Sevgili, dimethyl phthalate was found to be the carrier and water was determined to be the solvent ². The ternary diagram in the article presented equilibrium data at 298.15 K. The UNIQUAC data within the diagram was removed in order for the project data to be displayed more clearly.

Figure 1. Annotated sketch of a single stage LLX used to identify the given information and the unknowns that remain to be determined.



¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/jc1000022>.

*Foot note
not footer
:-2*

Formulate

The equations for the inverse Lever- Arm Rule (ILAR) and the Hunter Nash Graphical Method were used in the design and analysis of this project. The Hunter Nash method was essential in determining the number of equilibrium stages as requested in part B of the problem statement. The formulas for these methods are listed below.

Hunter Nash Method

$$F_i + S_i = M = E_i + R_i$$

$$R_n + E_n = R_{n+1} + E_{n+1}$$

Mixing Point

$$\frac{x_i^F F_i + x_i^S S_i}{F+S} = M$$

Analysis

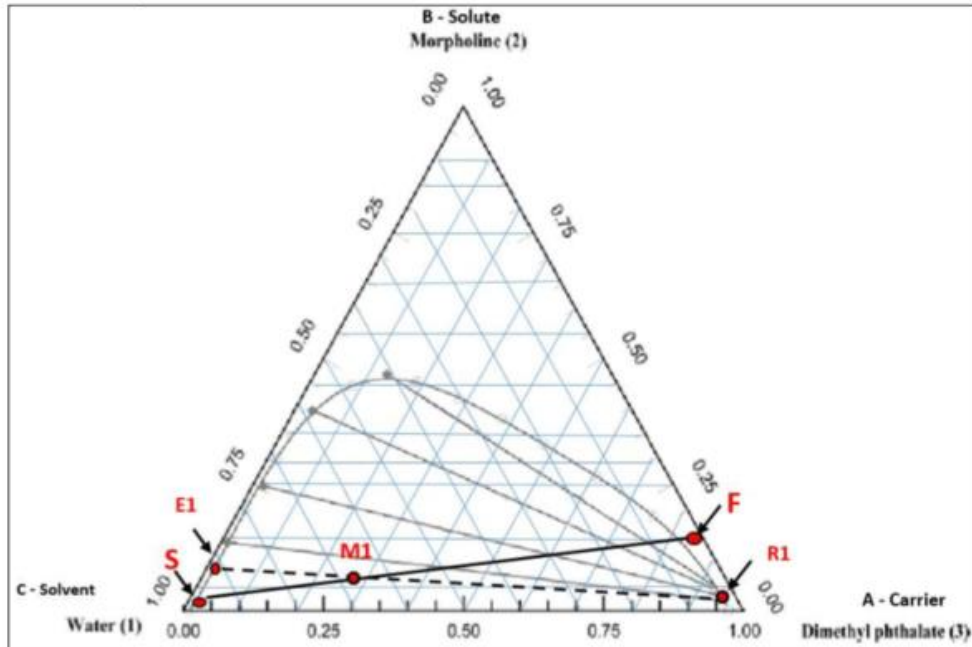
Part A

For part A, a single stage extraction method was used by first assuming a molar flow rate for the solvent feed for three different cases. Case 1 was for a solvent-feed (S/F) ratio of 2, meaning that the molar flow rate of the solvent stream would be double that of the molar flow rate for the feed stream. A basis of 1000 kmol/hr for the solvent stream was used and a molar flow rate of 500 kmol/hr for the feed stream. A material balance was performed and the mixing point equation was used in order to determine the composition of the mixing point. The calculations can be seen in Appendix A. The mixing point was then plotted on the ternary diagram along with the solvent and feed compositions. A line was drawn to connect all three points, representing the feed-solvent line or mixing line. A line was then drawn from one side of the equilibrium curve through the mixing point, in the opposite direction. This line was drawn in order to determine our raffinate and extract points. The feed-solvent line and raffinate-extract line must all pass through the mixing point. The extract point was placed on the left side of the diagram because the equilibrium tie lines displayed on the diagram are decreasing along the extract axis. This means that the partition coefficient is more than 1. The extract was found to have a composition of 0.06 for component B, the solute. The composition for each stream can be seen in Table 1. The ternary diagram for this is represented below in Figure 2.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/jc100002z>.

Figure 2. Ternary diagram for a single stage cascade displaying the feed, solvent, mixing extract, and raffinate points for case 1.

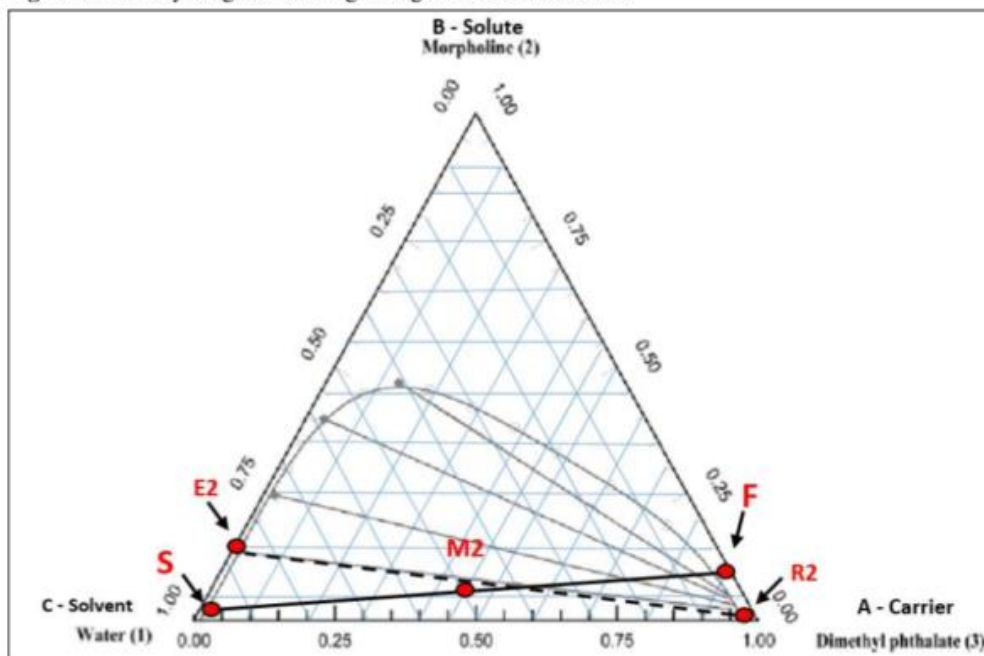


For case 2, a single stage unit with a S/F ratio of 1 and a molar flow rate of 500 kmol/hr for each of the entering streams was used. The mixing point for this case has compositions for component A and C that are much closer in value, hence moving the mixing point closer to a composition of 0.5 for both components. The solute composition in the mixing point does not change drastically because the composition of solute in the solvent stream is minuscule. Changing the S/F ratio to 1 and decreasing the molar flow rate of the solvent also increased the amount of component B in the extract stream to 0.10. The ternary diagram and composition of each stream for this case is displayed in Figure 3 and Table 1, respectively. In comparison to case 1, case 2 seemed to have the more ideal S/F ratio to increase the purity for x_B^E .

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/jc1000022>.

Figure 3. Ternary diagram for single stage cascade for case 2.

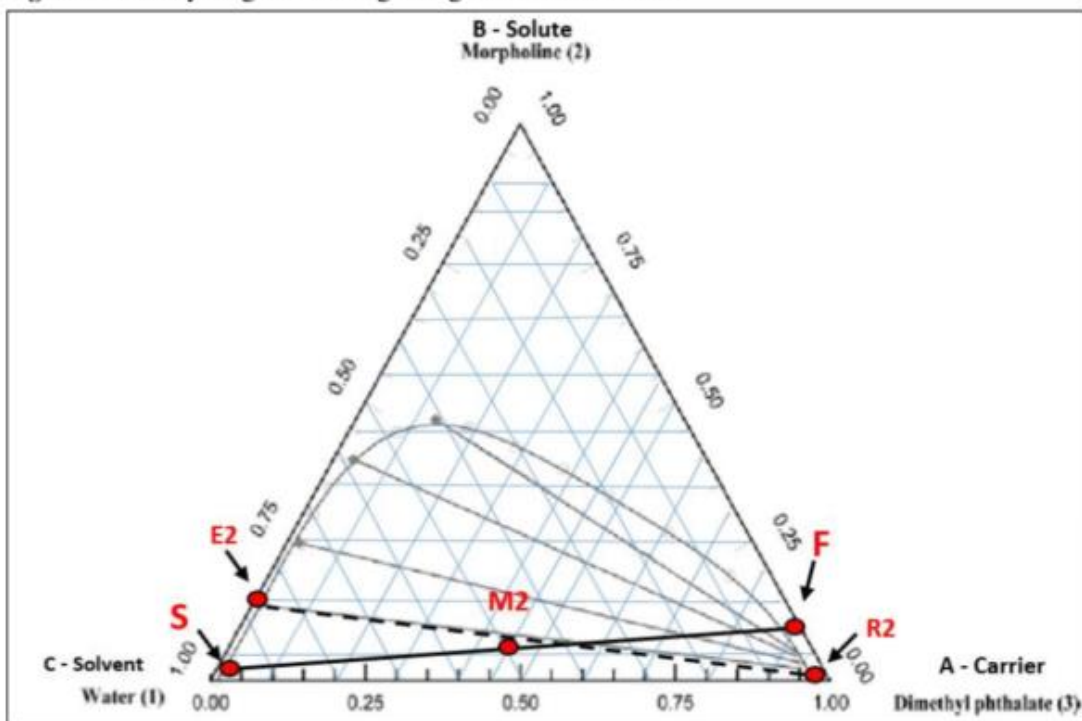


For case 3, a single stage unit was designed using a S/F ratio of 0.5. The molar flow rate of the feed used was 500 kmol/hr and the molar flow rate of the solvent was 250 kmol/hr. The compositions for all of the streams are displayed in Table 1. The ternary diagram for this case is displayed in Figure 4. Adjusting the S/F ratio increased the composition of B to 0.20 in the extract.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/jc1000022>.

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Table 1 - Composition of each stream for each of the three cases analyzed.

		Component A	Component B	Component C
Case 1	Mixing Point	0.30	0.04	0.66
	Extract	0.01	0.06	0.93
	Raffinate	0.92	0.04	0.04
Case 2	Mixing Point	0.45	0.05	0.50
	Extract	0.00	0.10	0.90
	Raffinate	0.99	0.00	0.01
Case 3	Mixing Point	0.60	0.07	0.33
	Extract	0.01	0.20	0.80
	Raffinate	0.99	0.00	0.10

Part B

For part B, we were assigned to make a counter-current cascade including the ternary diagram. We needed to determine the number of stages needed to achieve a product composition of 0.50 for component B in the extract. However, the desired purity would not be inside of the phase boundary curve. We began with an extract point composed of 0.45 for component B. This was the closest composition to 0.50. The feed flow rate used was 500 kmol/hr including compositions of 0.90 for A and 0.10 for B. We used the Hunter-Nash method to achieve the needed extract composition. We first found the mixing point using a material balance with a basis of 500 kmol/hr for the solvent stream. The operating point is then found by finding the intersection point of the F-E line and the S-R line. We then drew operating lines from the operating point that passed through the raffinate point to the second extract. We obtained a total of two stages. This is shown in Figure 3. A flow diagram of the cascade with the compositions for each stream are displayed in Figure 4.

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/jc1000022>.

Figure 3. A countercurrent cascade with multiple stages shown on a ternary diagram.

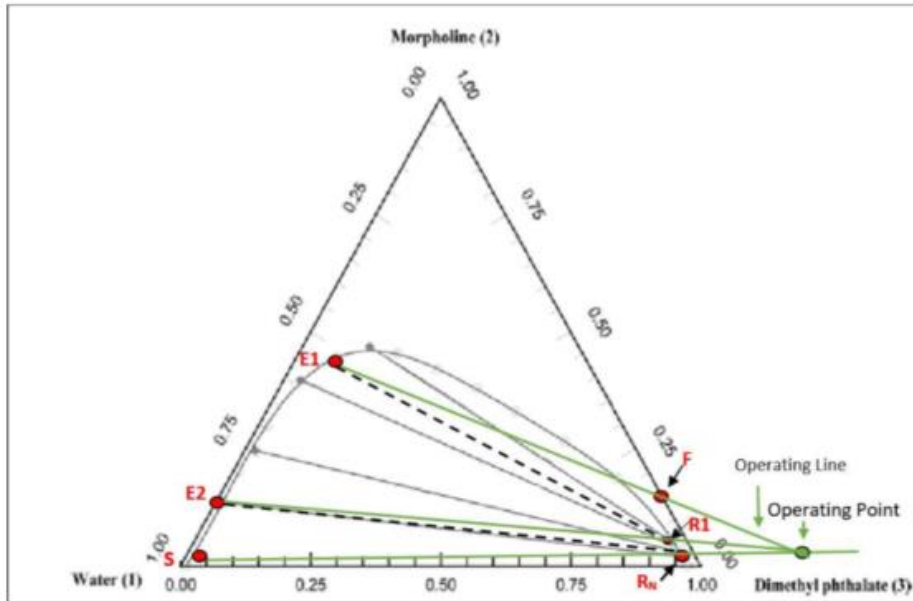
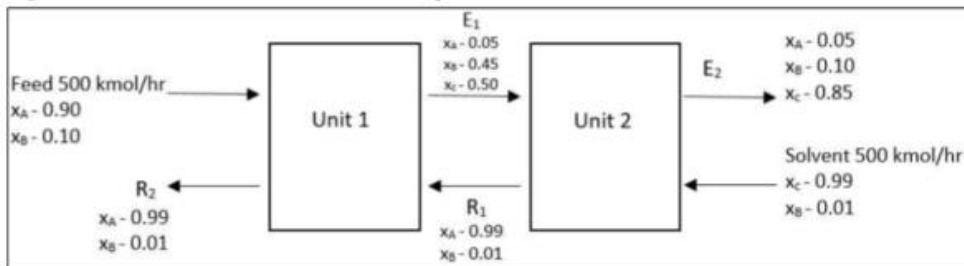


Figure 4. Countercurrent cascade with compositions of each stream.



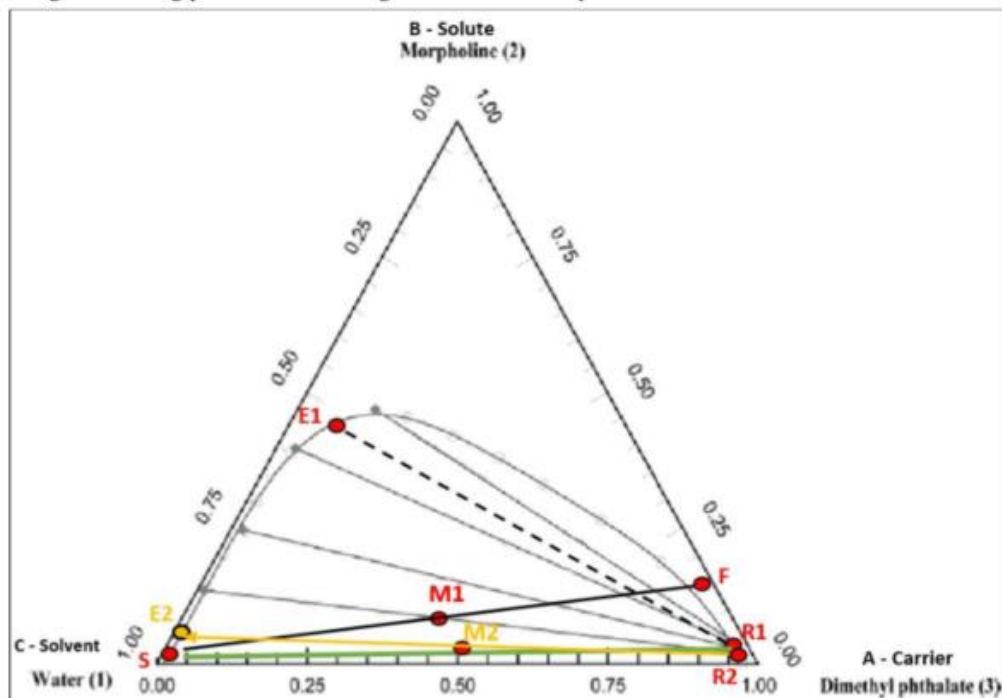
Part C

A crosscurrent extraction method was designed using two stages, the same amount of stages as those in the countercurrent method. A feed of 500 kmol/hr is fed to the first unit with a fresh

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

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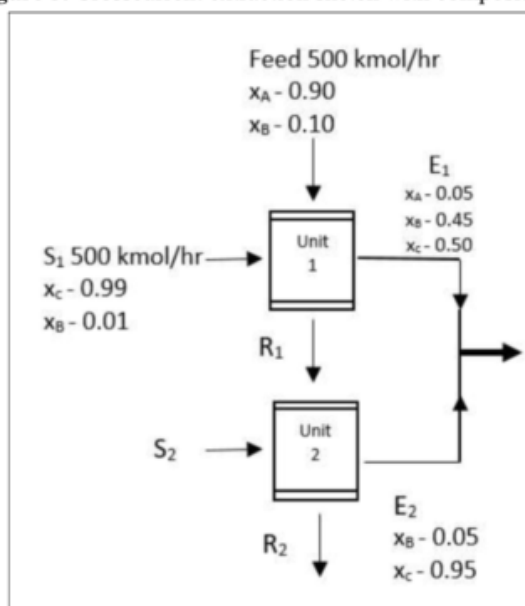
solvent stream fed to each unit. Again, the extract point selected includes a composition of 0.45 for component B, similar to the selected point in part B. To plot the ternary data, the feed-solvent line was drawn as in the previous sections. A line was drawn from the first solvent stream to the first raffinate, creating the second mixing point. The second extract-raffinate line was drawn using this mixing point and following the trend of the equilibrium tie lines.



¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed., (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/je1000022>.

Figure 5. Crosscurrent extraction sketch with compositions



Part D

Single stage extraction will either require a distillation unit in order to obtain a higher purity of the extract or will require an additional phase contact process to transfer a larger amount of solute. Crosscurrent extraction requires more solvent to be used, which can result in higher costs. Countercurrent and crosscurrent utilize numerous stages and thus can lead to a higher purity of the extract. Changing the solvent feed ratio does affect the composition of the product streams, increasing the purity when there is a S/F ratio less than 2. Overall, multi-stage systems and S/F ratios should be adjusted to increase purity of the solute in the extract stream.

Respectfully submitted,

Bryson Marshall

Zsamia Barnes

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/je1000022>.

Appendix A
Handwritten Calculations

Case 1: $F=500 \text{ kmol/hr}$ $S=1000 \text{ kmol/hr}$

Feed $\begin{cases} A = 0.90 (500 \text{ kmol/hr}) = 450 \text{ kmol/hr} \\ B = 0.10 (500 \text{ kmol/hr}) = 50 \text{ kmol/hr} \end{cases}$

Solvent $\begin{cases} B = 0.01 (1000 \text{ kmol/hr}) = 10 \text{ kmol/hr} \\ C = 0.99 (1000 \text{ kmol/hr}) = 990 \text{ kmol/hr} \end{cases}$

Total: $1000 + 450 + 50 + 10 + 990 = 1500 \text{ kmol/hr}$

Mixing Point:

$$A = (450 / 1500) \text{ kmol/hr} = 0.30 = A$$
$$B = [(50 + 10) / 1500] \text{ kmol/hr} = 0.04 = B$$
$$C = (990 / 1500) \text{ kmol/hr} = 0.66 = C$$

Case 2 $S/F=1$

Feed = 500 kmol/hr Solvent = 500 kmol/hr

Feed $\begin{cases} A = 450 \text{ kmol/hr} \\ B = 50 \text{ kmol/hr} \end{cases}$

Solvent $\begin{cases} B = 0.01 (500 \text{ kmol/hr}) = 5 \text{ kmol/hr} \\ C = 0.99 (500 \text{ kmol/hr}) = 495 \text{ kmol/hr} \end{cases}$

Total molar flow = 1000 kmol/hr

Mixing Point:

$$A = (450 / 1000) \text{ kmol/hr} = 0.45 = A$$
$$B = [(50 + 5) / 1000] \text{ kmol/hr} = 0.05 = B$$
$$C = (495 / 1000) \text{ kmol/hr} = 0.50 = C$$

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/jc1000022>.

Case 3 $S/F = 0.5$
Feed = 500 kmol/hr Solvent = 250 kmol/hr
Feed [$A = 450 \text{ kmol/hr}$
 $B = 50 \text{ kmol/hr}$
Solvent [$B = 0.01 (250 \text{ kmol/hr}) = 2.5 \text{ kmol/hr}$
 $C = 0.99 (250 \text{ kmol/hr}) = 247.50 \text{ kmol/hr}$
Total molar flow = 750 kmol/hr
Mixing Point:
 $A = (450/750) \text{ kmol/hr} = 0.60 = A$
 $B = (50 + 2.5)/750 \text{ kmol/hr} = 0.07 = B$
 $C = (247.5/750) \text{ kmol/hr} = 0.33 = C$

¹ Christie J. Geankoplis, A. Allen Hersel and Daniel. H. Lepek, *Transport Processes and Separation Process Principles* 5th ed. (Boston: Prentice Hall, 2018).

² Lutfullah M. Sevgili, Mehmet Bilgin, and Şahin Selin, "Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K," *Journal of Chemical & Engineering Data* 55, no. 9 (September 2010): pp. 3117-3120, <https://doi.org/10.1021/je1000022>.

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
SEPARATION PRCESS SPRING 2020**

Instructor: Dr. Nabila Shamim

Title of Assignment

TEST 1

Outcome Measured Using this Assignment

Outcome 1

An ability to identify, formulate, and solve **complex engineering problems** by applying principles of engineering, science, and mathematic.

OUTCOME 1.1 Ability to identify and formulate Separation problems using the principles of mathematics, engineering, and science.

Check the complex engineering problem characteristics related to this assignment

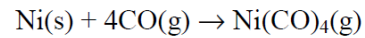
Assignment problem	
X	involves wide-ranging or conflicting technical issues,
	has no obvious solution
	Addresses problems not encompassed by current standards and codes
	involves diverse groups of stakeholders
X	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
	science
X	mathematics

Brief justification of why this assignment is suitable for this outcome

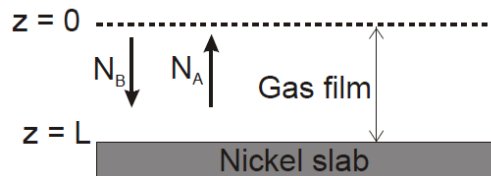
The questions on this section of Test 1 tests the students ability to identify relevant laws and equations, formulate the differential equation needed to solve the problem, and apply knowledge in mathematics to solve the resulting differential equations to solve mass transfer problems

Problem Statement & Grading Scheme

Problem 7 (a-d) (35 points) Nickel carbonyl (A) is produced by passing carbon monoxide (B) at 350 K and 1 atm over a nickel slab (catalyst bed) . 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

- List all the assumptions; simplify the general mass transfer equation for species A using stoichiometry of the reaction. **(5 Points)**

- b. Develop a concentration profile for the given system and specify your boundary conditions. **(6 Points)**

Ability of Formulate Engineering Problem

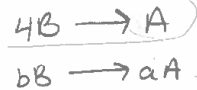
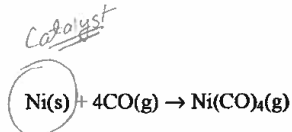
- c. Develop and formulate equation for the flux of species A. **(10 Points)**

Ability of solve Engineering Problem

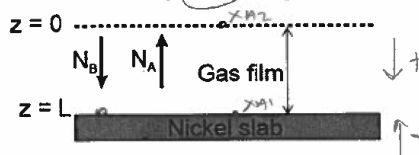
- d. Estimate the rate of production of nickel carbonyl (A), in $\text{mole/s}\cdot\text{cm}^2$ of solid surface at steady state. The composition of the bulk gas phase ($z = 0$) is 35 mol% CO. The binary diffusivity is $D_{AB} = 20.0 \text{ mm}^2/\text{s}$. **(10 Points)**
- e. What would be the rate of disappearance of carbon monoxide (B) in $\text{mole/s}\cdot\text{cm}^2$ **(4 Points)**

Sample Graded Student Work

Problem 7 (a-d) (35 points) Nickel carbonyl (A) is produced by passing carbon monoxide (B) at 350 K and 1 atm over a nickel slab (catalyst bed). 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.



$$P = P_A + P_B \Rightarrow P - P_B = P_A$$

Ability to Identify Engineering Problem

- a. List all the assumptions; simplify the general mass transfer equation for species A using stoichiometry of the reaction. (5 Points)

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

$$\frac{N_B}{b} = \frac{N_A}{-a} \Rightarrow N_B = -\frac{b}{a} N_A \Rightarrow N_B = \frac{4}{-1} N_A \Rightarrow \underline{N_B = -4N_A}$$

$$N_A = -D_{AB} \frac{dC_A}{dz} + \frac{C_A}{C_T} (N_A - 4N_A) ; \quad N_A = -D_{AB} \frac{dC_A}{dz} - \frac{C_A}{C_T} (3N_A)$$

$$\frac{dC_A}{dz} = \frac{dP_A}{RT} \therefore N_A = -\frac{D_{AB}}{RT} \frac{dP_A}{dz} - \frac{P_A}{P} (3N_A) \Rightarrow N_A + 3N_A \frac{P_A}{P} = -\frac{D_{AB}}{RT} \frac{dP_A}{dz}$$

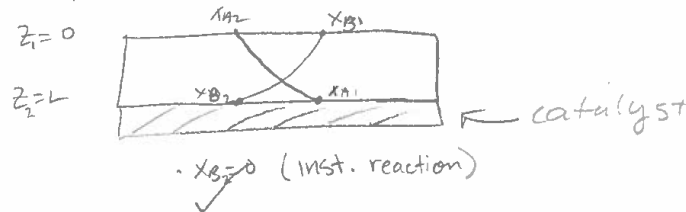
$$N_A \left(1 + \frac{3P_A}{P}\right) = -\frac{D_{AB}}{RT} \frac{dP_A}{dz}$$

$$N_A dz = \frac{-D_{AB}}{RT} \frac{dP_A}{\left(1 + \frac{3P_A}{P}\right)}$$

Assumptions:

- Instantaneous reaction
- Steady state
- Down is positive direction
- up is negative direction.

- b. Develop a concentration profile for the given system and specify your boundary conditions. (6 Points)



Ability to Formulate Engineering Problem

- c. Develop and formulate equation for the flux of species A. (10 Points)

$$N_A \int_{z_1}^{z_2} dz = - \frac{D_{AB}}{RT} \int_{P_{A2}}^{P_{A1}} \frac{dP_A}{\left(1 + \frac{3P_A}{P}\right)}$$

$$\rightarrow N_A z \Big|_{z_1}^{z_2} = \frac{D_{AB}}{RT} \int_{P_{A2}}^{P_{A1}} \frac{dP_A}{\left(1 + \frac{3P_A}{P}\right)} \quad \leftarrow \text{(Switch Limits to get positive \pm)}$$

$$\rightarrow N_A \underbrace{(z_2 - z_1)}_L = \frac{D_{AB}}{RT} \int_{P_{A2}}^{P_{A1}} \frac{dP_A}{\left(1 + \frac{3P_A}{P}\right)} \quad ; \quad \text{u-substitution} \rightarrow u = 1 + \frac{3P_A}{P} \quad ; \quad du = \frac{3}{P} \cdot dP_A$$

$$dP_A = \frac{P}{3} \cdot du$$

$$\rightarrow N_A = \frac{D_{AB}}{RTL} \int \frac{\frac{P}{3} \cdot du}{u} \Rightarrow N_A = \frac{D_{AB} P}{3RTL} \left[\ln \left(1 + \frac{3P_A}{P} \right) \right]_{P_{A2}}^{P_{A1}}$$

$$\rightarrow N_A = \frac{D_{AB} \cdot P}{3RTL} \left[\ln \left(1 + \frac{3P_{A1}}{P} \right) - \ln \left(1 + \frac{3P_{A2}}{P} \right) \right] \Rightarrow N_A = \frac{D_{AB} P}{3RTL} \ln \left(\frac{\left(1 + \frac{3P_{A1}}{P} \right)}{\left(1 + \frac{3P_{A2}}{P} \right)} \right)$$

$$\rightarrow N_A = \frac{D_{AB} \cdot P}{3RTL} \ln \left[\left(\frac{P + 3P_{A1}}{P} \cdot \frac{P}{P + 3P_{A2}} \right) \right] \Rightarrow N_A = \frac{D_{AB} \cdot P}{3RTL} \ln \left(\frac{P + 3P_{A1}}{P + 3P_{A2}} \right)$$

$\uparrow$
 $P_{A2} = P$
 $(P_{B2} = 0)$

5 $\rightarrow N_A = \frac{D_{AB} P}{3RTL} \ln \left(\frac{P + 3P_{A1}}{4P} \right)$

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
SEPARATION PROCESS SPRING 2020**

Instructor: Dr. Nabila Shamim

Title of Assignment

Exam 2

Outcome Measured Using this Assignment

Outcome 1

An ability to identify, formulate, and solve **complex engineering problems** by applying principles of engineering, science, and mathematic.

Outcome 1.2

Ability to solve complex distillation problems using science, and mathematic.

Check the complex engineering problem characteristics related to this assignment

Assignment problem	
	involves wide-ranging or conflicting technical issues,
X	has no obvious solution
	Addresses problems not encompassed by current standards and codes
	involves diverse groups of stakeholders
X	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
	science
X	mathematics

Brief justification of why this assignment is suitable for this outcome

Exam 2 identifies students ability to solve complex separation process problems using graphing tools. Using McCabe-Thiele method to calculate distillation problems

Problem Statement & Grading Scheme

Separation Process CHEG 3043 PO 2 (Spring 2020):

Exam 2 Time: 2 Hrs Date: April 22, 2020

Total points: 100

STUDENT NAME:DATE:

Open Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO COLLABORATION

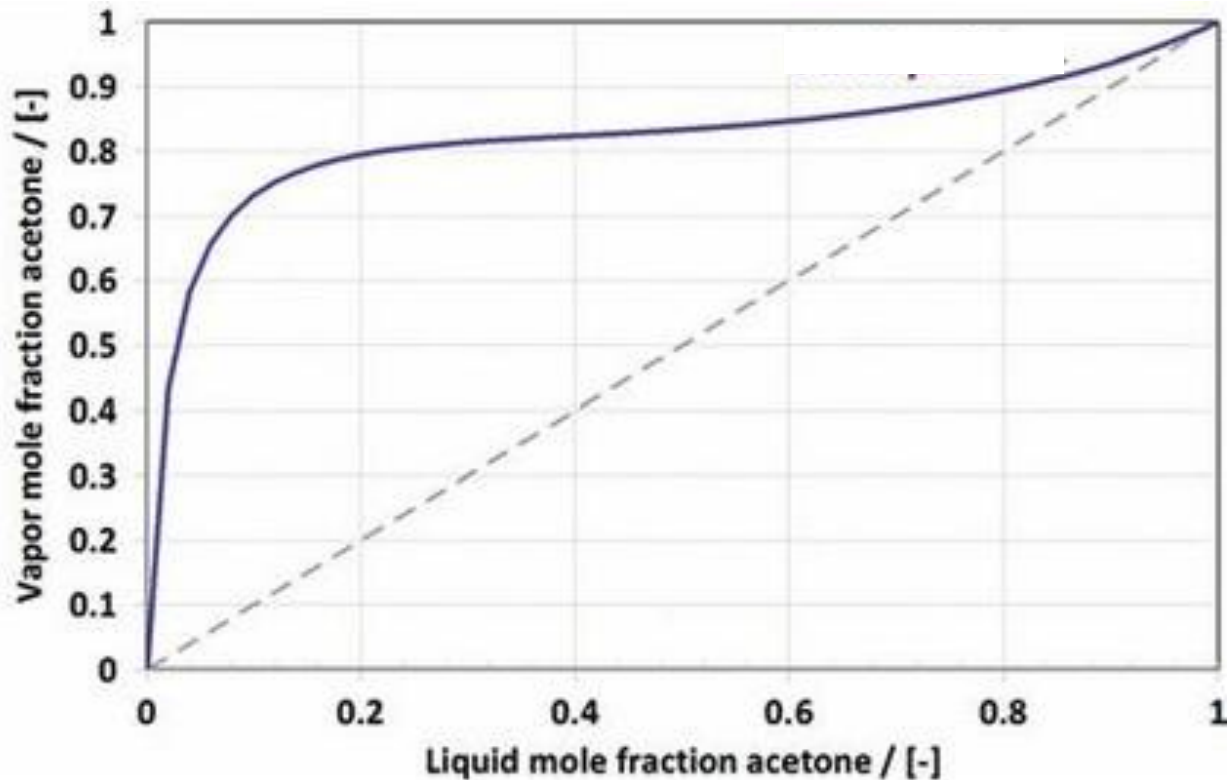
PROVIDE UNITS ON ALL CALCULATIONS AND ANSWERS

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

Student Signature:

Problem 1 (55 Points) Acetone is removed from aqueous streams by distillation. The feed contains 10 mol% acetone. The distillate must have a purity of at least 95 mol % and the aqueous effluent must not contain more than 1 mole % acetone. The feed enters the column as saturated liquid.

1. Draw a schematic diagram of the process and label all the parts of the distillation column 10 Points
2. Calculate Minimum number of theoretical stages N_m 15 Points
3. Calculate Minimum reflux ratio R_{min} 10 points
4. Develop the equation for the rectification column 10 points
5. Estimate the number of ideal stages required (you can use a schematic diagram and then show your steps how to estimate the no of stages). 10 points



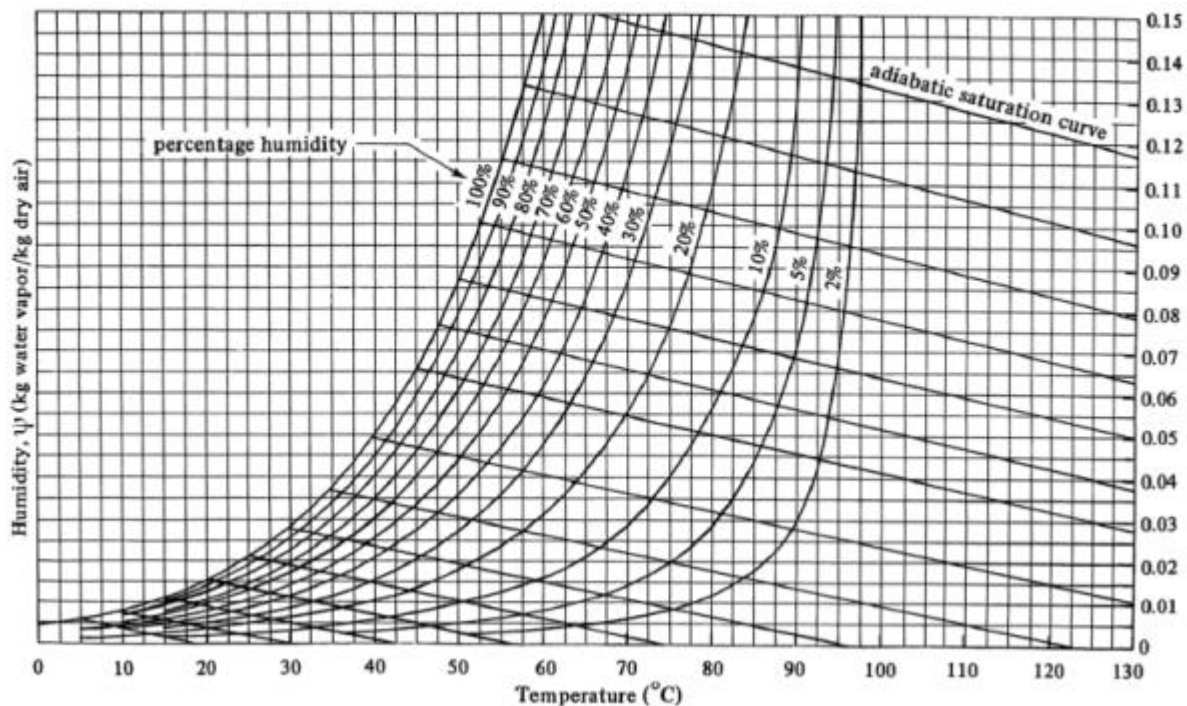
Problem 2. (25 Points) Calculate the feed line slope for the following two cases

- A two phase feed where 75 % of the feed is vaporized under column conditions
- A liquid feed subcooled by 35oF, given the average liquid heat capacity is 30 Btu/lbmol oF and latent heat is 15000 Btu /lbmol.
- Draw schematic diagram of the effect of feed condition on the feed tray for the above two cases.

Problem 3. (20 Points) An air stream at 70oC and carrying 0.055 kg water per kg dry air is adiabatically contacted with liquid water until it reaches equilibrium. The process is continuous and operating at steady state.

- What is the percent humidity of the incoming air stream?
- What is the percentage humidity of the air stream leaving?
- What is the humidity [mas/mass] of the air stream leaving
- What is the temperature of the air stream leaving?

Psychrometric chart



Sample Graded Student Work



CHEG 3043 Test 2
Chiebuka Ejimadu.pdf

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
SEPARATION PROCESS SPRING 2020**

Instructor: Dr. Nabila Shamim

Title of Assignment

Final Project

Outcome Measured Using this Assignment

Outcome 1

An ability to identify, formulate, and solve **complex engineering problems** by applying principles of engineering, science, and mathematic.

Outcome 1.2

Ability to solve complex Absorption and distillation engineering problems using computing tools.

Check the complex engineering problem characteristics related to this assignment

Assignment problem	
X	involves wide-ranging or conflicting technical issues,
X	has no obvious solution
	Addresses problems not encompassed by current standards and codes
X	involves diverse groups of stakeholders
	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
	science
X	mathematics

Brief justification of why this assignment is suitable for this outcome

The project tests the students ability to solve complex separation process problems using graphing and computing tools. Using Aspen - HYSIS develop a simple process

Problem Statement & Grading Scheme

Final Project CHEG 3043

This is a group project. The project is **due on May 1, 2020**.

Also upload the completed project in Task stream under **Assignment (Outcome 1)**

Odd Groups : A conceptual design for the production of Methanol.

Even Groups: A conceptual design for the production of Ethyl Benzene.

For both Odd and Even Group

- a. At least 95% purity of product is required and the bottom must not have more than 1 % of the product.
- b. Estimate the number of ideal stages required number of minimum stage
- c. Estimate the number of ideal stage for feed entry
- d. Composition profile as a function of theoretical tray
- e. Temperature profile as a function of theoretical tray

Use literature to find more information on the reactor and the detail process for separation using ASPEN.

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.

Having zoom update meetings with the instructor will help to keep the project stay on track. A detailed project rubric is given below.

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** (5) – 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. **Introduction** (10)
Application and need of the product. Different methods that can be used for the synthesis of the product. Finally the recommended method used for your project.
4. **Methods** (30)
 - I. Steady State process simulation (10)
 - a. Basic Equipment
 - b. Input specification data summarized in table
 - c. include any data and physical property values obtained or estimated from the literature with references in tabular form
 - d. Mass and Energy Balance
 - e. The desired heating and cooling mediums
 - f. Desired operating temperature
 - g. Desired operating pressure range
 - II. Reaction Kinetics (10)
 - a. Write all the equations to produce the product
 - b. Condition of the reactants
 - c. Conditions of product going into separation units
 - III. Process Simulation.(10)
 - a. ASPEN Flow sheet of design
 - b. Column sizing detail

5. Process Simulation and results (30)

- a) Primary Control objectives such as reboiler heat input, reflux ratio
- b) Recycle stream properties
 - Acceptable composition
 - Is further processing required?
- c) The graphs or figures you have obtained from Aspen HYSYS.
 - Estimate the number of ideal stages required number of minimum stage
 - Estimate the number of ideal stage for feed entry
 - Composition profile as a function of theoretical tray
 - Temperature profile as a function of theoretical tray
- d) Output requirements
 - Desired end prproduct specifications
 - Purity requirements

6. Recommendations for further development/ Things that can go wrong during the process (10)

7. Conclusions. (5)

8. References (5)

Confedential Feedback of group member

All groups need to send me their HYSYS project via email

Do not attach the entire Aspen HYSYS results printout

Sample Graded Student Work



52534_Paul_Danjuma
_final_report_1549171

**OUTCOME “1” SPECIFIC ASSIGNMENTS
USED TO ASSESS THE OUTCOME IN**

**KINETICS AND REACTOR DESIGN
SPRING 2020**

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
KINETICS AND REACTOR DESIGN CHEG 3063 Y01
SPRING 2021
Instructor: Dr. NABILA SHAMIM**

Title of Assignment

Exam 2

Outcome Measured Using this Assignment

Outcome 1.1 Identify and Formulate engineering problems using principles of engineering

Brief Description of the suitability of this assignment for the outcome

Identify and Formulate reaction problems using principles of engineering/mathematics/science

Kinetics and Reactor Design CHEG 3063 PO 1 (Spring 2021):

Exam I Time: 1Hr 20 min Date: April 21, 2021

Instructor: Dr. Nabila Shamim

Total points: 100

ABET OUTCOME 1 An ability to identify, formulate and solve complex engineering problem by applying principle of engineering science and mathematics.

STUDENT NAME:DATE:

Competency area	Points	Score earned
Outcome 1.1 Identify and formulate (i) Understand the given problem and identify the subject area and concepts involved a. Derive rate law and net rates and selectivity b. Combine all equation to solve	50	
2.1 Concept problems	50	
Total	100	

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 EXAMS 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 (50 Points) The liquid phase irreversible multiple reactions are carried out isothermally in a PFR



Species A is a limiting reactant and species D and U are desired and undesired products respectively. The inlet (feed) concentration of A is 1 (mol/L) and inlet concentration of B is 1 (mol/L) after mixing ($C_{A0}= C_{B0}= 1$ (mol/L)).

The outlet concentrations (mol/L)

$$C_A = 0.05$$

$$C_B = 0.02$$

$$C_D = 0.55$$

$$C_U = 0.25$$

- What is the type of these multiple reactions? (5 points)
- Does the rate law of there reactions follow the elementary or non-elementary? How can we decide it? (5 Points)
- Complete the rate law of these multiple reactions. (Given rates, net rates for each species, relative rates for each reaction and each species) (20 Points)
- What is the instantaneous selectivity and instantaneous yield at the outlet? (10 Points)
- What is the overall selectivity and overall yield at the outlet? (10 Points)

Problem 2 (Multiple Choices)

1. What is the concentration of B for the isothermal gas phase reaction $A + 2B \longrightarrow 3C$ in PFR given that the rate law appears to be elementary and $F_{A0} = 0.01$ mol/min and $F_{B0} = 0.01$ mol/min? Show your work. **5 points**

a. $C_B = C_{A0}(1 - X) \frac{P}{P_0}$

b. $C_B = C_{A0} \frac{(1-X)P}{(1+X)P_0}$

c. $C_B = C_{A0}(1 - 2X) \frac{P}{P_0}$

d. $C_B = C_{A0} \frac{(1-2X)P}{(1+2X)P_0}$

e. None of the above

2. For a constant volume batch reactor in which component A reacts to form B, what is the reaction order when $\ln(C_{A0}/C_A)$ is found to linear with time t? **5 points**

a. 0th order

b. 1st order

c. 2nd order

d. 3rd order

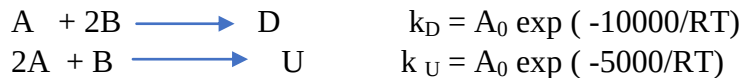
e. None of the above.

3. For the parallel elementary reactions below, what would you do to maximize the production of D? Show your work. **5 points**



- a. Use a PFR and /or decrease the temperature.
b. Use a CSTR and /or decrease the temperature.
c. Use a PFR and/or increase the temperature
d. Use a CSTR and /or increase the temperature.
e. Use a membrane reactor semipermeable to U

4. Parallel multiple reactions



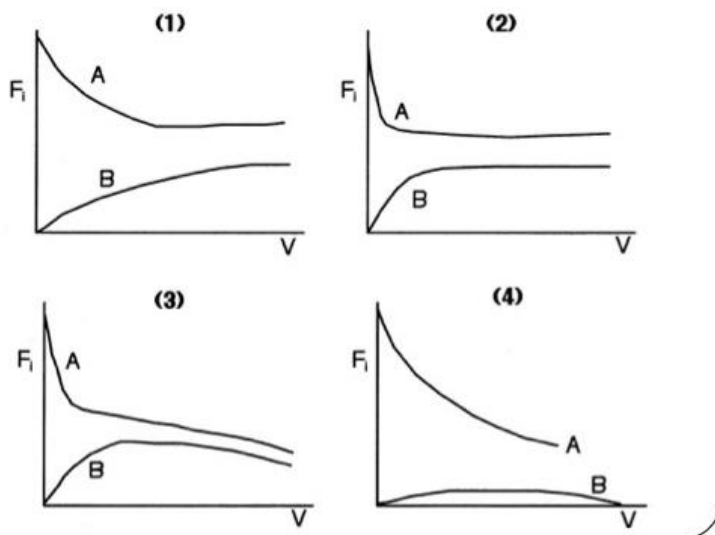
To maximize the instantaneous selectivity ($S_{D/U}$) what would you do? List all that apply. Assume elementary irreversible reactions and A_0 is the same. Show your work. (10 points)

- Use a CSTR
 - Use a PFR
 - Use a semi batch reactor with stream B flowing in
 - Use a semi batch reactor with stream A flowing in
 - Increase temperature
 - Decrease temperature
5. For the elementary series reactions, $\text{A} \xrightarrow{\quad} \text{B} \xrightarrow{\quad} \text{C}$, the net production of B is given by, **5 points**

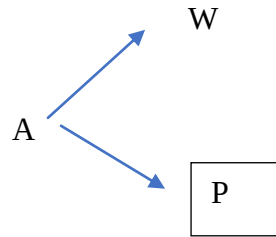
- $r_B = k_1 C_A$
- $r_B = k_1(C_A - C_B/K_C)$
- $r_B = k_1 C_A - k_2 C_B$
- $r_B = -k_1 C_A + k_2 C_B$
- $r_B = k_1 C_A - k_2(C_B - C_C/K_C)$

(show your work)

6. $2\text{A} \rightleftharpoons \text{B} + \text{C}$ Which of the following are membrane reactor and why? **5 points**



- 1 and 2
 - 3 and 4
 - 2 and 3
 - 4 and 1
7. Consider the reaction network below, if the overall selectivity of W to P is 0.4, what is the overall yield? Show your work. **5 points**



- a. 0.2
- b. 0.75
- c. 0.8
- d. 4.0

8. For the isothermal elementary gas phase reaction $2A \rightarrow B$ how does the PFR volume required for a given conversion change with increasing mole fraction y_{A0} of A if the inlet concentration of A and inlet total volumetric flow rate remain constant? There is no ΔP .
(10 Points)

Bonus Problem (5 Points) Given the elementary irreversible liquid phase reaction

$2A + 2B \longrightarrow 3C$ what is the Damkohler number (Da) for CSTR? Show your work.

- a. τk
- b. $\tau k C_{A0}$
- c. $\tau k C_{A0}^2$
- d. $\tau k C_{A0}^3$
- e. $\tau k C_{A0}^4$



Exam 2 best.pdf

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
KINETICS AND REACTOR DESIGN CHEG 3063 Y01
SPRING 2021**

Instructor: Dr. NABILA SHAMIM

Title of Assignment

Assignment 3

Outcome Measured Using this Assignment

Outcome 1.2

**Identify and Formulate reaction engineering problem using
MATLAB/POLYMATH**

Brief Description of the suitability of this assignment for the outcome

Identify and Formulate Reaction engineering problem multiple reactions.

Chemical Reaction Kinetics and Reactor Design CHEG 3063 YO 1 (Spring 2021):
Assignment 3 Due Date: April 10, 2021

STUDENT NAME:DATE:

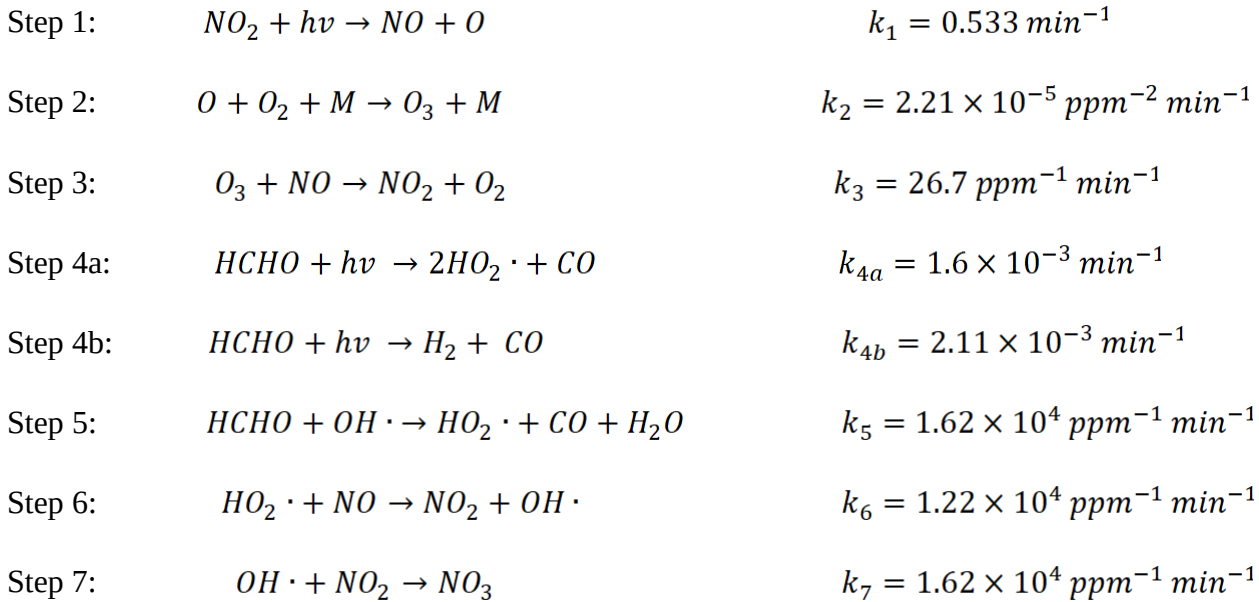
Open Book Assignment

Upload the graded homework in task stream under Outcome1Multiple Reactions (use Polymath)

Student Signature:

Problem Statement

A seven step mechanism can be used to describe the atmospheric reactions involving formaldehyde and nitrogen oxides at 1 atm and T=298 °C as presented by Seinfeld. These photochemical reactions lead to the formation of ozone:



The photolysis reactions of step 1, 4a and 4b are written for the case where the incoming solar radiation is assumed to be constant at the midday value of k_{iM} thus leading to the given rate constants. Where, $h\nu = h * \nu$ the Incoming solar radiation, photolysis reaction rate constants

$h = 6.626 \times 10^{-34}$ Plank's Constant; m²

kg/s

$\nu = c / \lambda$ # Frequency

$c = 3 \times 10^8$ Speed of light, m/s and

$\lambda = 4 \times 10^{-7}$ Wavelength of Visible Light, m.

A more detailed model would be to have the rate constants for these steps vary with the time of the day according to

$$k_i = k_{iM} \sin \left[\frac{2\pi(t - 6)}{24} \right] \text{ for } \sin \left[\frac{2\pi(t - 6)}{24} \right] > 0 \quad [\text{Equation 1}]$$

$k_i = 0$ for all other values of t

Where t is the time in hours on a 24 hours/day basis and the solar radiation begins at 6 am and ends at 6 pm.

All of the reactions in the mechanism are considered to be elementary as written. For example, the rate of the second step is given by:

$$r_2 = k_2 C_O C_{O_2} C_M$$

Where the concentrations are in ppm. C_M is the concentration of third bodies, which is considered to be at a constant value of 10^6 ppm and C_{O_2} the concentration of oxygen is constant at 0.21×10^6 ppm.

The simplest applications of chemical engineering to urban smog simulation involves considering the atmosphere below an inversion layer to be a batch reactor with no input or output terms. The resulting material balance for each of the species in the mechanism can be made and expressed as ordinary differential equations. Thus for ozone:

$$\frac{dC_{O_3}}{dt} = k_2 C_O C_{O_2} C_M - k_3 C_{O_3} C_{NO}$$

Similar material balances can be made for the other reacting components, including the free radicals. Typical initial conditions for all free radicals are that the concentrations are essentially zero.

Consider a simplified model for photochemical smog that is represented by seven step mechanism for formaldehyde.

- A. Find the concentration profiles for O_3 , NO_2 , NO , and $HCHO$ for the given initial conditions and the constant values of photolysis reaction rate constants of step 1, 4a, and 4b.
- B. Repeat part a for a single 24 hour day starting at midnight with the same initial conditions but with the three photolysis reactions varying according to the general relationship of equation 1.



Assignment best.pdf

**OUTCOME SPECIFIC ASSIGNMENTS
USED TO ASSESS OUTCOMES**

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
KINETICS AND REACTOR DESIGN CHEG 3063 Y01
SPRING 2021
Instructor: Dr. NABILA SHAMIM**

Title of Assignment

Assignment 2

Outcome Measured Using this Assignment

Outcome 2.1

Ability to Define/Understand the Kinetics and reactor design Problem

Brief Description of the suitability of this assignment for the outcome

Clearly defines the design strategy and methodology. Identifies and breaks down work into tasks and subtasks and identifies the personnel and deliverables for each when required

please upload the homework in task stream under **Assignment (Outcome - 2)**

Problem 1. The catalytic gas phase reaction $A \longrightarrow B$ to be carried out in a packed bed reactor under isothermal operation. The reactant is pure A with an inlet concentration of 1 g-mol/dm³, the entering pressure is 25 atm and the entering volumetric flow rate is 1 dm³/min. the first order reaction rate constant K, which is based on reactant A is 1 dm³/kg.cat. min.

1. Develop the chemical reaction engineering algorithm, - mole balance, rate laws stoichiometry and combine them together, finally solve the following using MATLAB.
2. Study the effect of the pressure drop on the conversion for the first order reaction and plot conversion and pressure ($p = P/P_0$) as a function of the weight of the packing material W. consider the pressure drop parameter α is between 0.05 – 0.2 /kg. also consider the maximum weight of the catalyst is 2 kg.

Problem 2 The dehydrogenation of a compound (elementary kinetics) is taking place in a selective membrane reactor under isothermal conditions.



The reaction is reversible and K_c is the equilibrium constant. The manner in which K_c (the mass transfer coefficient at volumetric flow rate v_0) increases with flow rate depends upon the flow geometry and the mass transfer dependence on velocity is given by

$$K_c = k_{co} (v/v_0)^{1/2}$$

And the membrane transport of C is given by $k_c \alpha C_c$ when permeate concentration of C is low.

The following parameter values apply,

$$k = 0.5 \text{ dm}^3/\text{kg.min}, \quad v_0 = 50 \text{ dm}^3/\text{min}, \quad K_c = 0.5 (\text{kg-mol/dm}^3)^{-1/2}$$

$$P_0 = 10 \text{ atm}, \quad F_{Ao} = 10 \text{ kg-mol/min}; \quad \alpha = 0.002 \text{ atm/kg}$$

$$K_{co} = 0.1 \text{ dm/min} \quad W = 200 \text{ kg}$$

1. Compare the calculated output valued of FB, the molar flow rate of B for no pressure drop.



Assignment
Outcome 2.1 Best.pdf

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
KINETICS AND REACTOR DESIGN 3063 Y01
SPRING 2021**

Instructor: Dr. NABILA SHAMIM

Title of Assignment

Final Project Report

Outcome Measured Using this Assignment

Outcome 2.3

Ability to perform detailed design of complex chemical engineering design

Brief Description of the suitability of this assignment for the outcome

Identifies applicable codes and standards for the design. Performs all relevant detailed analysis (engineering, mathematical, economic) in accord with applicable codes and standards. Develops complete final design specifications.

Final Project CHEG 3063
Spring 2021 Due Date April 30, 2021

Project objectives:

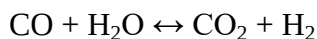
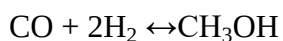
- To demonstrate your understanding of designing a packed bed reactor.
- Show that you can calculate the required design taking heat, pressure drop and changing physical properties into account.
- Design and create a plan of action that you will follow to achieve your goal.
- To reflect afterwards on your group's progress and judge how you followed your plan.

You are required to design a shell and tube packed-bed reactor for methanol synthesis. The complete problem statement follows.

1. Projects are to be tackled in groups, with one report per group. Each student will submit at the end of the project a confidential assessment of the relative contributions of the members of the group.
2. The methodology used in the design of the reactor must be clearly explained; all assumptions must be identified and evaluated; the results must be clearly presented and discussed. In particular you must have a section at the start of your report where you: "clearly explain the strategy you will follow to achieve the project's objective". Use bullet points showing the sequence of steps you planned.
3. Reports must be written in an acceptable and professional style and should not exceed 15 typed pages (including any appendices). Any polymath code you choose to include in part of your page limit. You must submit your report using Canvas.
4. All published information consulted must be appropriately referenced.
5. At the end you must have a section called "Reflection". Answer these 3 questions in the section:
 - How accurately did our group stick to the plan (there is no penalty from deviating from your plan, but describe why you deviated).
 - How would we go about the project differently if we could redo it?
 - What did we learn from doing this project (bullet points are OK).

Problem statement

A new catalyst has been proposed for the synthesis of methanol from carbon monoxide and hydrogen gas. This catalyst is reasonably active between temperatures of 330 K to about 430 K. The reactions to be considered are:



The reactions are elementary and occur in a reactor containing tubes packed with a precious metal catalyst on a silica support. Heat is removed from the reactor by generating steam on the shell side of the tubes. The feed consists of 7/15 hydrogen gas, 1/5 carbon monoxide, 1/5 carbon dioxide, and 2/15 steam. The total flow rate is 300 mol.s⁻¹. The entering pressure may be varied between 1 atm and 160 atm and the entering temperature between 300 K and 400 K. A total tubular reactor volume of 2 m³ is to be used.

The following tasks should be completed:

1. Discuss the commercial application of this reaction in terms of the overall process, economics, process conditions, reactor types and configurations typically used, type of catalyst, typical conversion and end product usage.
2. Assuming isothermal and isobaric conditions, determine the entering conditions of temperature and pressure that will optimize the production of methanol. Hint: Do this by conducting several simulations at discrete combinations of T_0 and P_0 . First try $T_0 = 330$ at $P_0 = 40$ atm, then try $T_0 = 380$ and $P_0 = 1$ atm)
3. Carry out a detailed reactor design of a shell and tube reactor for the optimal feed conditions determined in part 2. Pressure drop and non-isothermal effects are to be taken into account.

The shell side temperature can be controlled by adjusting the steam pressure and may be assumed constant at a value specified by you. Physical property estimation sources, techniques and assumptions should be clearly presented. The design should include the following:

- the reactor dimensions and number of tubes
 - the reactor conditions; including composition, pressure and temperature profiles (as a function of reactor length).
 - A mechanical sketch of the reactor should be included.
 - **Not required:** mechanical design of the reactor, including specification of the reactor material of construction, shell and tube wall thickness and capital cost for the design.
4. Determine the effect of variations in:
 - ratio of feed H_2 to CO ,
 - ratio of feed H_2O to CO ,
 - assumed heat transfer coefficient, U
 5. All results must be presented in SI units throughout the report.

The following results should be tabulated in your report:

Inlet temperature [K]

Outlet temperature [K]

Inlet pressure [Pa]

Outlet pressure [Pa]

Maximum tube-side temperature [K]

Location from inlet of maximum temperature [m]

Methanol production rate [kg.s⁻¹]

Reactor length [m]

Total inlet concentration, CT0 at 330K

Rate constant, k1 at 330K

Equilibrium constant KC,1 at 330K

Rate constant, k2 at 330K

Equilibrium constant KC,2 at 330K

Heat of reaction for reaction 1 at 330K

Heat of reaction for reaction 2 at 330K

The following results for Reactor in and Reactor out in a tabular form must be presented

Flow [mol.s⁻¹]

Pressure [Pa]

Temperature [K]

CO (mole fraction)

H2

CO2

CH3OH

H2O

If you are using MATLAB, A working set of MATLAB files must be emailed to the instructor with submission of your final report. These MATLAB files must generate the final profiles used to obtain the flows, pressure, temperature and mol fractions in the above tables. Non-working code, or code that does not lead to the values in the table will lead to a penalty in the grade.

Additional problem information Thermodynamic and rate data T is in Kelvin, but $R = 1.987 \text{ cal.mol}^{-1} .\text{K}^{-1}$. The subscript 1 refers to the methanol reaction, while subscript 2 refers to the water-gas shift reaction. $V = 40 \text{ dm}^3$

$$K_1 = 131667(0.001987T)^2 \exp \left[\frac{30620}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right] \left[\frac{\text{dm}^3}{\text{mol}} \right]^2$$

$$K_2 = 103943 \exp \left[\frac{9834}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right]$$

$$k_1 = 0.933 \times 10^{-6} \exp \left[2.5 \left(\frac{31400}{R} \left(\frac{1}{330} - \frac{1}{T} \right) \right) \right] \left[\left(\frac{\text{dm}^3}{\text{mol}} \right)^2 \text{s}^{-1} \right]$$

$$k_2 = 0.636 \times 10^{-6} \exp \left[\frac{18000}{R} \left(\frac{1}{300} - \frac{1}{T} \right) \right] \left[\frac{dm^3}{mol.s} \right]$$



Final project
chad.pdf

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
KINETICS AND REACTOR DESIGN**

SPRING 2020

Instructor: Dr. Nabila Shamim

Title of Assignment

Exam 2

Outcome Measured Using this Assignment

Outcome 1

An ability to identify, formulate, and solve **complex engineering problems** by applying principles of engineering, science, and mathematic.

Outcome 1.2

Ability to solve the reaction engineering/mathematical/science formulations analytically, numerically

Check the complex engineering problem characteristics related to this assignment

Assignment problem	
	involves wide-ranging or conflicting technical issues,
X	has no obvious solution
	Addresses problems not encompassed by current standards and codes
	involves diverse groups of stakeholders
X	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
	science
X	mathematics

Brief justification of why this assignment is suitable for this outcome

The questions in Test 3 test the student's ability to identify relevant laws and equations, formulate the solution methodology, and solve the resulting engineering equations for the Reaction Engineering. Test 3 also tests the student's ability to perform analysis Using Polymath - Identify and Formulate multiple reaction problems using principles of engineering/mathematics/science. The problem has no obvious solution since assumptions need to be made.

Exam 2 Time: 24 Hrs Date: April 23, 2020
Exam ends at 8 PM Friday
Total points: 100

STUDENT NAME:DATE:

Open Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO COLLABORATION

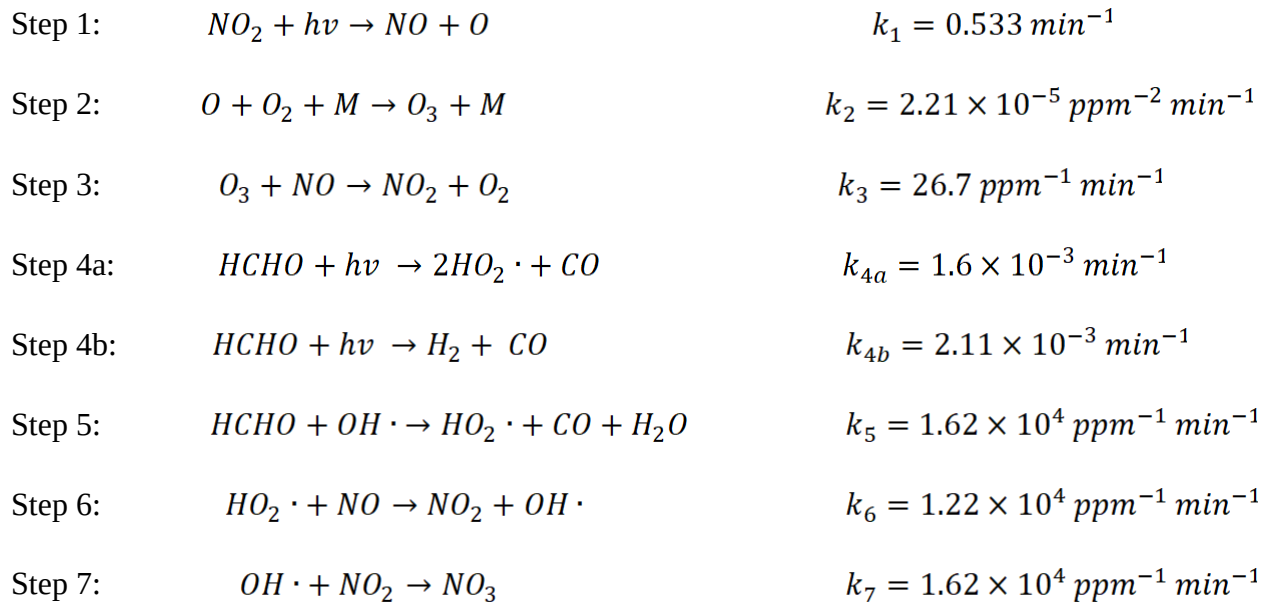
PROVIDE UNITS ON ALL CALCULATIONS AND ANSWERS

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

Student Signature:

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The photolysis reactions of step 1, 4a and 4b are written for the case where the incoming solar radiation is assumed to be constant at the midday value of k_{iM} thus leading to the given rate constants. Where, $h\nu = h \cdot \nu$ the Incoming solar radiation, photolysis reaction rate constants

$h = 6.626 \times 10^{-34}$ Plank's Constant; m²

kg/s

$\nu = c / \lambda$ # Frequency

$c = 3 \times 10^8$ Speed of light, m/s and

$\lambda = 4 \times 10^{-7}$ Wavelength of Visible Light, m.

A more detailed model would be to have the rate constants for these steps vary with the time of the day according to

$$k_i = k_{iM} \sin \left[\frac{2\pi(t - 6)}{24} \right] \text{ for } \sin \left[\frac{2\pi(t - 6)}{24} \right] > 0 \quad [\text{Equation 1}]$$

$k_i = 0$ for all other values of t

Where t is the time in hours on a 24 hours/day basis and the solar radiation begins at 6 am and ends at 6 pm.

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The simplest applications of chemical engineering to urban smog simulation involves considering the atmosphere below an inversion layer to be a batch reactor with no input or output terms. The resulting material balance for each of the species in the mechanism can be made and expressed as ordinary differential equations. Thus for ozone:

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Similar material balances can be made for the other reacting components, including the free radicals. Typical initial conditions for all free radicals are that the concentrations are essentially zero.

Consider a simplified model for photochemical smog that is represented by seven step mechanism for formaldehyde.

- A. Find the concentration profiles for O_3 , NO_2 , NO , and $HCHO$ for the given initial conditions and the constant values of photolysis reaction rate constants of step 1, 4a, and 4b.

- B. Repeat part a for a single 24 hour day starting at midnight with the same initial conditions but with the three photolysis reactions varying according to the general relationship of equation 1.

Rubric for the Exam 2

Assumptions for Reaction (5 points)

Given Information (5 Points)

Formulation (35 Points)

Mole Balance Rate Law Rate related with mole balance Solving (35 Points) Show all differential equations, explicit equations conditions used for solving. Using Polymath Program part, A Using Polymath Program Part B Results (20 Points) Polymath results in tabular form part A Polymath results graphical presentation part A Polymath results in tabular form part B Polymath results graphical presentation part B Comparison of Results for part A and part B for the above-mentioned concentration

Sample Graded Student Work



Kinetics Exam
2-DT.pdf

**OUTCOME “1” SPECIFIC ASSIGNMENTS
USED TO ASSESS THE OUTCOME IN**

**EQUILIBRIUM STAGED
SEPARATION PROCESSES**

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
CHEG 3043 P01 SEPARATIONS
SPRING 2020**

Instructor: Dr. Irvin W. Osborne-Lee

Title of Assignment

**EXERCISE – DISTILLATION OF BENZENE AND
TOLUENE (VARIATIONS ON TEXTBOOK EXAMPLE)**

Outcome Measured Using this Assignment

Outcome 1

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

Check the complex engineering problem characteristics related to this assignment

Assignment problem	
	involves wide-ranging or conflicting technical issues,
X	has no obvious solution
	Addresses problems not encompassed by current standards and codes
	involves diverse groups of stakeholders
X	includes many component parts or sub-problems
	involves multiple disciplines
	has significant consequences in a range of contexts
Assignment problem involves the application of the principles of	
X	engineering
	science
	mathematics

Brief justification of why this assignment is suitable for this outcome

The goals in the Final Project allow students to demonstrate an ability to identify relevant principles, theories, methods and tools, formulate the an approach needed to solve the problem, and apply knowledge of thermodynamics, graphical methods, and computer simulation to achieve elements of distillation column design

Problem Statement & Grading Scheme

Sample Graded Student Work

Khristen Liverman

CHEG 3043 Equilibrium Staged Separation Processes
Binary Fractional Distillation Column Design

Practice Problem (Exercise)
Tuesday 7 April 2020

Upload to eCourses for quiz grade.
Show your work for full credit.

98/100

Problem Statement

For the example shown (see 5th edition shown below, or 4th edition Example 11-4.1), rework the problem for two cases. Case I: the reflux ratio is increased by 10%. Case II: the reflux ratio is reduced by 10%. Compare the results for these two cases to those for the problem as originally presented in the textbook.

EXAMPLE 26.4-1. Rectification of a Benzene-Toluene Mixture

A liquid mixture of benzene-toluene is to be distilled in a fractionating tower at 101.3 kPa pressure. The feed of 100 kg mol/h is liquid, containing 45 mol % benzene and 55 mol % toluene, and enters at 327.6 K (130°F). A distillate containing 95 mol % benzene and 5 mol % toluene and a bottoms containing 10 mol % benzene and 90 mol % toluene are to be obtained. The reflux ratio is 4:1. The average heat capacity of the feed is 159 kJ/kg mol · K (38 btu/lb mol · °F) and the average latent heat 32099 kJ/kg mol (13 800 btu/lb mol). Equilibrium data for this system are given in Table 26.1-1 and Fig. 26.1-1. Calculate the kg moles per hour distillate, kg moles per hour bottoms, and the number of theoretical trays needed.

The table and figure below are the corresponding ones from the 4th edition.

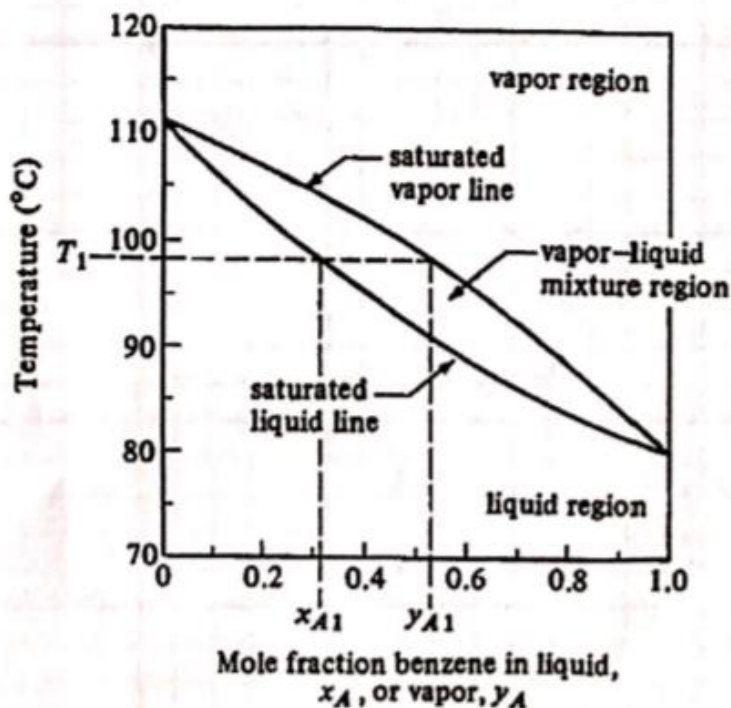


FIGURE 11.1-1. Boiling point diagram for benzene (A)-toluene (B) at 101.325 kPa (1 atm) total pressure.

Identify:

liquid mixture

Benzene [A]

Toluene [B]

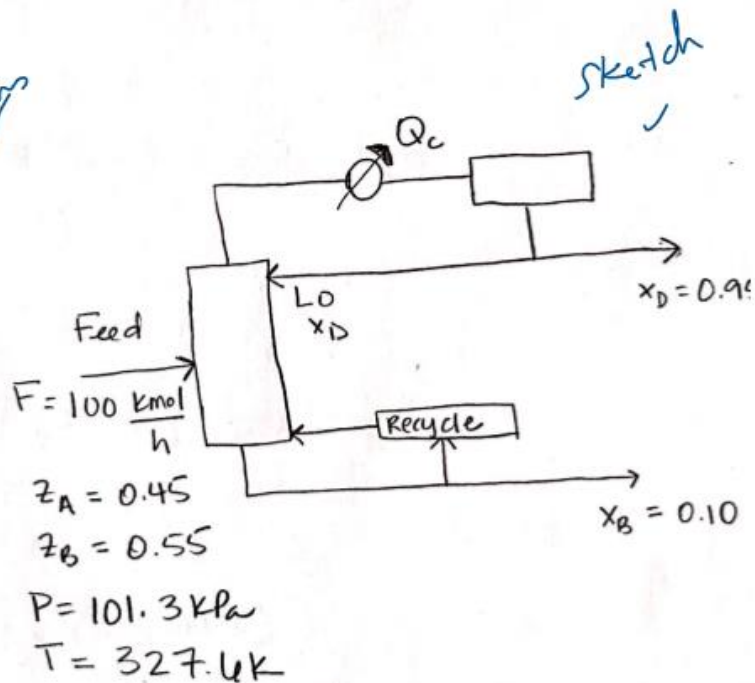
reflux ratio: $\frac{4}{1}$

$C_{PL} = 159 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}$

average latent heat: $H_V - H_L$

$32099 \frac{\text{kJ}}{\text{kmol}}$

Given



Find:

D. $\frac{\text{kmol}}{\text{h}}$

CASE I: Reflux ratio: $\frac{4.4}{1}$ *See graph

B. $\frac{\text{kmol}}{\text{h}}$

CASE II: Reflux ratio: $\frac{3.6}{1}$

Goals ✓

Formulate:

Compare, too! — 2.

rectifying operating line: $y_2 = \frac{x_D}{(R+1)} + x_1 \frac{R}{(R+1)}$, $R = \frac{L_0}{D}$

stripping operating line: $y_B = x_N \frac{R_B+1}{R_B} - \frac{x_B}{R_B}$, $R_B = \frac{V'}{B}$

q-line operating line: $q = \frac{L' - L}{F} = \frac{\hat{H}_V - \hat{H}_F}{\hat{H}_V - \hat{H}_L}$, $y = \frac{q}{q-1} x - \frac{z_F}{q-1}$

$$\hat{H}_V - \hat{H}_F = (\hat{H}_V - \hat{H}_L) + (\hat{H}_L - \hat{H}_F)$$

$$\hat{H}_L - \hat{H}_F = C_{PL} (T_B - T_F)$$

key equations ✓

Total mass balance: $F = D + B$

Component mass balance: $z_F F = x_D D + x_B B$

Solve: case I

$$F = D + B$$

$$100 \frac{\text{kmol}}{\text{h}} = D + B \rightarrow B = 100 - D$$

$$z_A F = x_D D + x_B B$$

$$(0.45)(100) = (.95)(D) + (.10)(100 - D)$$

$$45 = .95D + 10 - .10D$$

$$35 = .85D$$

$$D = 41.2 \text{ kmol/h}$$

∴

$$B = 100 - 41.2 = 58.8 \text{ kmol/h} = B$$

$$q = \frac{\hat{H}_V - \hat{H}_F}{\hat{H}_V - \hat{H}_L} = \frac{(\hat{H}_V - \hat{H}_L) + (\hat{H}_L - \hat{H}_F)}{(\hat{H}_V - \hat{H}_L)} = \frac{(\hat{H}_V - \hat{H}_L) + C_{PL}(T_B - T_F)}{(\hat{H}_V - \hat{H}_L)}$$

From txy graph @ $z_A = 0.1$

$$q = \frac{32099 \frac{\text{kJ}}{\text{kmol}} + 159 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}} [365.65 \text{ K} - 327.6 \text{ K}]}{32099 \text{ kJ/kmol}} = 1.188 = q$$

$$y = \frac{1.188x}{1.188-1} - \frac{0.45}{1.188-1} \rightarrow y = 6.3x - 2.4$$

$$0 = 6.3x - 2.4$$

$$2.4 = 6.3x \rightarrow x = 0.38$$

Points for q-line

$$(0.38, 0), (0.45, 0.45)$$

$$y_2 = \frac{0.95}{(4.4+1)} + x_1 \frac{4.4}{(4.4+1)} \rightarrow y_2 = 0.175 + x_1 (.815)$$

$$y_2 = 0.175 + (0)(.815)$$

$$y_2 = 0.175$$

Points for rectifying line

$$(0, .175), (0.95, 0.95)$$

8 stages

7 trays

Solve: case II

$$D = 41.2 \text{ kmol/h}$$

$$B = 58.8 \text{ kmol/h}$$

$$q = 1.188, y = 6.3x - 2.4$$

} not effected by reflux ratio

$$y_2 = \frac{.75}{(3.6+1)} + x_1 \frac{3.6}{(3.6+1)} = y_2 = 0.206 + x_1 (.782)$$

$$y_2 = 0.206 + (0)(0.782)$$

$$y_2 = 0.206$$

points for rectifyline (0, 0.206), (0.95, 0.95)

8 stages

7 trays

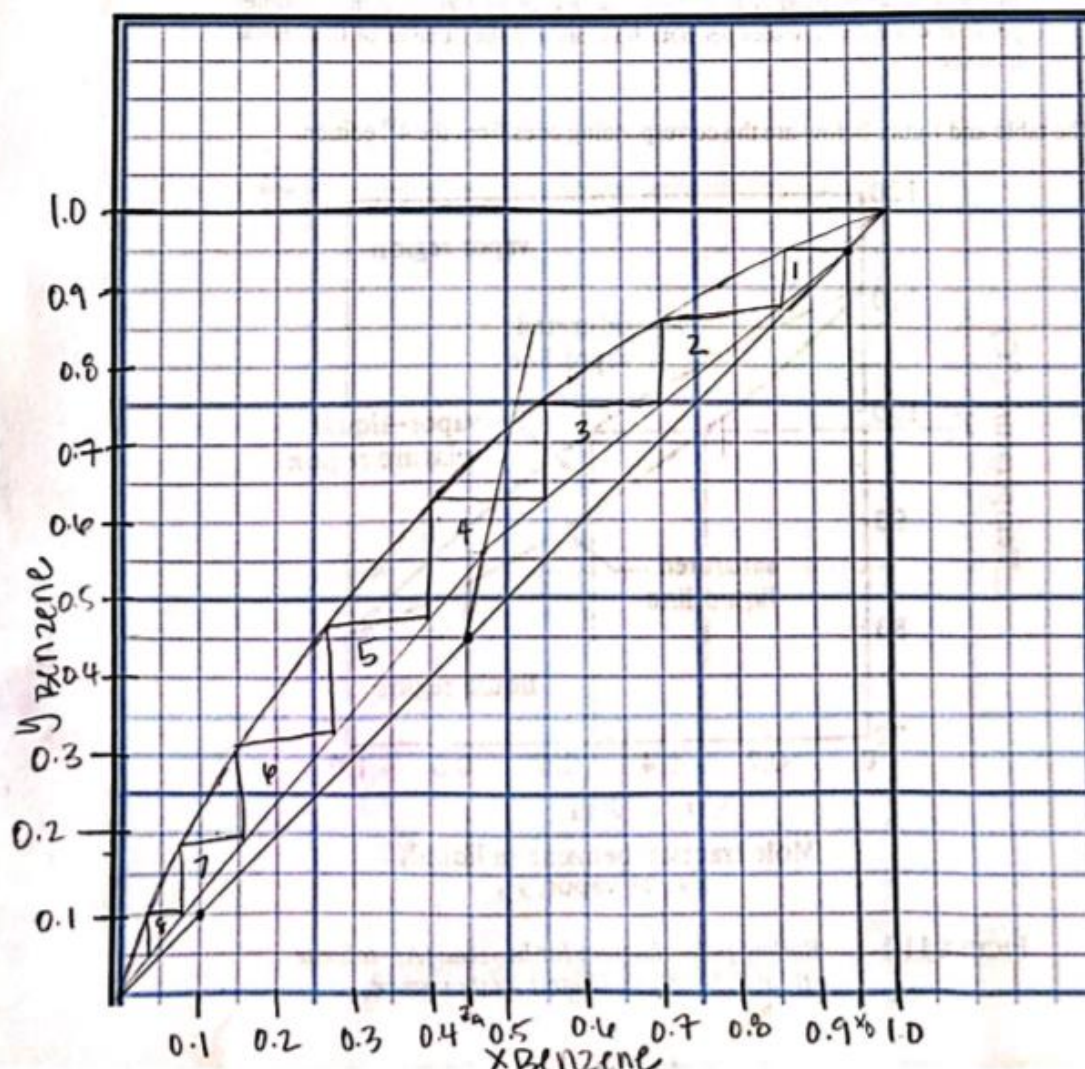
Discussion

Increasing or decreasing the reflux by 10% does not change the amount of trays that are needed. *compare*

Case I

TABLE 11.1-1. Vapor-Pressure and Equilibrium-Mole-Fraction Data
for Benzene-Toluene System

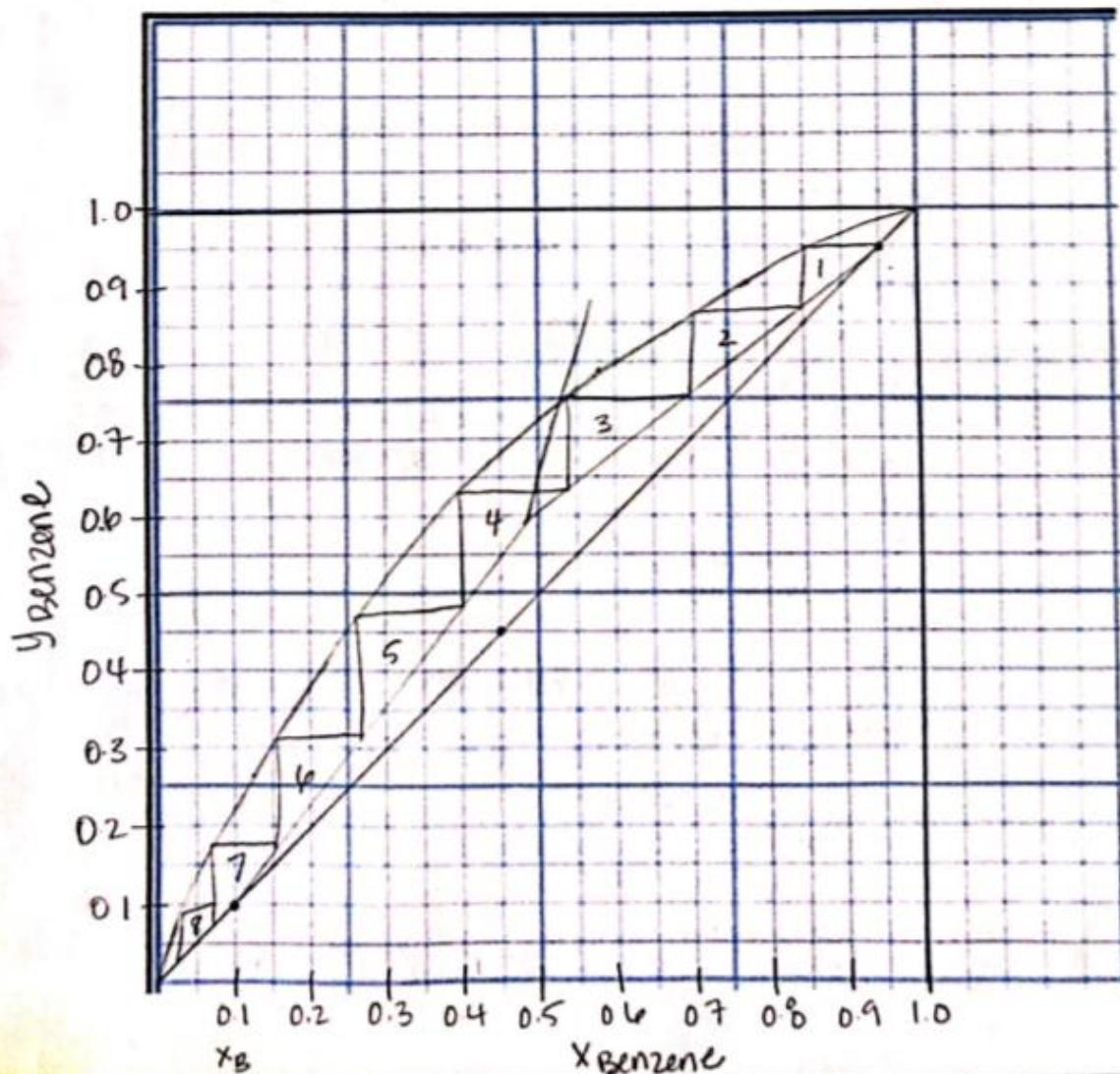
Vapor Pressure							
Temperature		Benzene		Toluene		Mole Fraction Benzene at 101.325 kPa	
K	°C	kPa	mm Hg	kPa	mm Hg	x_A	y_A
353.3	80.1	101.32	760			1.000	1.000
358.2	85	116.9	877	46.0	345	0.780	0.900
363.2	90	135.5	1016	54.0	405	0.581	0.777
368.2	95	155.7	1168	63.3	475	0.411	0.632
373.2	100	179.2	1344	74.3	557	0.258	0.456
378.2	105	204.2	1532	86.0	645	0.130	0.261
383.8	110.6	240.0	1800	101.32	760	0	0



Case II

TABLE 11.1-1. Vapor-Pressure and Equilibrium-Mole-Fraction Data for Benzene-Toluene System

Vapor Pressure							
Temperature		Benzene		Toluene		Mole Fraction Benzene at 101.325 kPa	
K	°C	kPa	mm Hg	kPa	mm Hg	x_A	y_A
353.3	80.1	101.32	760			1.000	1.000
358.2	85	116.9	877	46.0	345	0.780	0.900
363.2	90	135.5	1016	54.0	405	0.581	0.777
368.2	95	155.7	1168	63.3	475	0.411	0.632
373.2	100	179.2	1344	74.3	557	0.258	0.456
378.2	105	204.2	1532	86.0	645	0.130	0.261
383.8	110.6	240.0	1800	101.32	760	0	0



**OUTCOME “1” SPECIFIC ASSIGNMENTS
USED TO ASSESS THE OUTCOME IN**

**EQUILIBRIUM STAGED
SEPARATION PROCESSES**

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
CHEG 3043 P01 SEPARATIONS
SPRING 2020**

Instructor: Dr. Irvin W. Osborne-Lee

Title of Assignment

**FINAL PROJECT:
Distillation Column Design with HYSYS**

Outcome Measured Using this Assignment

Outcome 1

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Problem Statement & Grading Scheme

Sample Graded Student Work

CHEG 3043 **Equilibrium Staged Separation Processes**
Binary Fractional Distillation Column Design

Project (*Final Exam Weight*)
Tuesday 14 April 2020

Team Based Project – Distillation Column Design Using HYSYS Due Thursday 7 May 2020

Answer all questions. You will be graded based on your ability to use the techniques, skills, and modern engineering tools necessary for engineering practice. You are to work in **ENGLISH ENGINEERING UNITS**. Failure to do work in English engineering units will result in the loss of 50 % of the points. Clarity of presentation is essential if you are to avoid losing points. NOTE: This is a team assignment.

You are to separate up to 1,000 lbmol/h (but not less than 500 lbmol/h) of a binary mixture as assigned in the table below into a liquid distillate of 99 mol % of light key (or MVC - most volatile component) and a liquid bottoms product of 98 mol % heavy key (or LVC - least volatile component). The feed is a saturated liquid at 55 psia and the column operates at a pressure in the reflux drum of 18 psia. A total condenser is used to obtain saturated liquid reflux and liquid distillate at its bubble point. A partial reboiler is used at the bottom of the column to produce vapor boilup and a saturated liquid bottoms product.

MVC (Normal boiling point (°C))	LVC (Normal boiling point (°C))	Relative volatility		
		Team #	Optimal	High
Benzene (80.1)	Toluene (110.6)	2.27	2.34	2.40
Toluene (110.6)	<i>p</i> -Xylene (138.3)	Team 7	2.31	2.44
Benzene (80.6)	<i>p</i> -Xylene (138.3)	4.25	4.82	5.75
<i>m</i> -Xylene (139.1)	<i>p</i> -Xylene (138.3)	1.0201	1.0202	1.0204
Pentane (36.0)	Hexane (68.7)	Team 1	2.59	2.79
Hexane (68.7)	Heptane (98.5)	Team 2	2.45	2.64
Hexane (68.7)	<i>p</i> -Xylene (138.3)	6.54	7.00	7.32
Ethanol (78.4)	iso-Propanol (82.3)	Team 3	1.17	1.19
iso-Propanol (82.3)	<i>n</i> -Propanol (97.3)	Team 4	1.78	1.84
Ethanol (78.4)	<i>n</i> -Propanol (97.3)	Team 5	2.10	2.22
Methanol (64.6)	Ethanol (78.4)	Team 8	1.56	1.71
Methanol (64.6)	iso-Propanol (82.3)	Team 6	2.26	2.33
Chloroform (61.2)	Acetic Acid (118.1)	5.20	6.15	8.40
Acetone (56.2)	Propylacetate (101.7)	4.50	4.74	5.05

Using the handout and HYSYS, (1) run a short-cut distillation and (2) model the continuous steady state distillation. (3) Also use the graphical McCabe Thiele method using a y-x diagram done by hand (using the system assigned to your team in Table above) to compare and plot the Txy diagram. You may want to start with activity (3).

You already know how to do item(3). A set of standard operating procedures (SOP) are included in this package that will guide you in setting up the HYSYS simulations for activities (1) and (2). Present your results in the form of a letter report, with those findings from activities (1), (2) and (3) presenting the following in A WELL FORMATTED AND CLEARLY LABELED TABLE:

- (a) The bubble point temperature of the feed
- (b) The minimum reflux ratio
- (c) The minimum number of trays
- (d) The actual number of trays
- (e) The optimal feed stage
- (f) The external reflux ratio?
- (g) The molar flow rates of the distillate and the bottoms
- (h) The condenser and reboiler duties, and
- (i) The bubble point temperatures and pressures of the distillate and bottoms respectively

You already have your team assignments.

Simulating Distillation Columns with HYSYS

- Click START
- Click ASPEN-HYSIS
- Click FILE
- Click NEW
- Click CASE (Ctrl + N)
- Master Component List appears below SIMULATION BASIS MANAGER Header Bar
- Click Fluid Pkg (to the Right of Components in the Lower Bar)
- Click ADD
- Click EOS (Equation/s Of State)
- Under property Package Filter select Activity Models
- Click/Select the appropriate Activity Model that best fits your system
- To the right of Component List Selection, Click VIEW
- Either scroll down to the components to be selected or write the name of component in the box to the right of MATCH, and then Click ADD PURE
- Repeat for each component
- Close windows and return to the Basis Manager
- Click on Enter Simulation Environment
- Click on Tools to enable the selection of appropriate units
- Click Preferences
- Click Variables
- Click Field to use English engineering units and SI to work in SI units
- Close window to return to PFD- case
- Define the Feed stream by Clicking on the blue arrow and place it in the green area
- Double click on the stream and specify it by naming it as F (for feed)
- Specify two of the following three in the worksheet: Vapor fraction, Temperature and Pressure; Vapor fraction = 0 means the liquid is at its bubble point ; Vapor fraction = 1 means vapor at its dew point
- Specify P and T when the Feed (stream) is a sub-cooled liquid or a superheated vapor
- Specify either the total Molar or Mass flow rate
- Click Composition and specify either the mole or mass fraction or either the molar or mass flow of each component. Note that if you specify the component mole or mass flows, you DO NOT have to specify the total molar or mass flow (choose the option that requires fewer calculations on your part)

SHORT-CUT DISTILLATION

- You must first run a short-cut distillation (as in the McCabe-Thiele method) to find out the number of equilibrium stages (HYSYS actually gives an approximate value of the Actual Number of Trays) and the feed tray location
- Pick the icon for the short-cut distillation (square column with condenser and reboiler)
- Place the icon in the drawing area and double click on it
- In the Window that appears select the Feed stream and write F (for feed) as specified above
- Enter NAMES ONLY for the energy streams, that is name the Condenser as Qc-100 and the Reboiler as Qr-101
- Enter NAMES ONLY of the streams for the DISTILLATE as D-100 and the REBOILER as B-101
- Select the phase of the top product (LIQUID for total condenser and VAPOR for partial condenser)
- Click on PARAMETERS
- Enter the LIGHT KEY component and its MOLE FRACTION in the BOTTOMS PRODUCT
- Enter the HEAVY KEY component and its MOLE FRACTION in the DISTILLATE
- The CONDENSER and REBOILER pressures are then specified as follows
- Specify the pressures in the CONDENSER and REBOILER you know you will use or as given in the problem statement
- The REBOILER pressure must be EQUAL to or GREATER than the CONDENSER, so that the VAPORS can FLOW up the COLUMN
- Immediately, the CONDENSER and REBOILER pressures are specified, the SIMULATOR (HYSYS) will then give you the MINIMUM REFLUX RATIO
- You MUST then specify an EXTERNAL REFLUX RATIO
- A GOOD RULE OF THUMB is to start with an EXTERNAL REFLUX RATIO 1.2 times the MINIMUM REFLUX RATIO
- Click on the PERFORMANCE Tab to see the results of the Short-cut distillation calculation done by HYSYS
- If the condenser temperature as given by the short-cut calculation is too low ($< 100^{\circ}\text{F}$), you must go back and raise the pressure; this may also require raising the EXTERNAL REFLUX RATIO
- If the REBOILER temperature is too high ($> 450^{\circ}\text{F}$), you must go back and lower the pressures
- HYSYS now gives you the required number of equilibrium stages (labeled ACTUAL NUMBER OF TRAYS)
- Go BACK and ADJUST the REBOILER pressure by applying the RULE OF THUMB to specify the REBOILER pressure HIGHER THAN the CONDENSER pressure by allowing 0.75kPa (Ref. Peters et al., Plant Design and Economics for Chemical Engineers, page 968) or 0.1088 psi drop per TRAY
- After obtaining reasonable temperatures, and the correct pressures, record the following as calculated by HYSYS
- The ACTUAL NUMBER OF TRAYS at the specified EXTERNAL REFLUX RATIO
- The OPTIMAL FEED STAGE
- The EXTERNAL REFLUX RATIO from the DESIGN Tab in the PARAMETERS Window
- The DISTILLATE molar flow from the Worksheet Tab

Rigorous Distillation (Modeling Continuous Steady State Distillation)

- Pick icon for rigorous distillation (that is the icon which has a Column with Condenser and Reboiler) and place it in the drawing area (you need not delete the column for the short-cut distillation)
- Double Click on it to open it
- Enter the number of PLATES
- Select TOP DOWN to start numbering the stages from the top
- Name your Feed/inlet stream (e.g. F-200; different from what you used for the short-cut distillation)
- Enter the Condenser type: TOTAL REFLUX = Liquid Distillate; PARTIAL REFLUX = Liquid and Vapor Distillates, and FULL REFLUX = Vapor Distillate
- Name your Distillate stream (e.g., D-200), and your Bottoms stream (e.g., B-201) – NAMES ONLY
- Name your Condenser and Reboiler duties (e.g., Qc-200 and Qr-201 respectively) – NAMES ONLY
- Click anywhere in the Screen and the NEXT button will appear in Bold indicating you can move to the next step
- If NEXT is not active, HYSYS will tell you what else needs to be specified
- Click on NEXT (if it is active and appears as described)
- On the NEXT window specify the pressure(s) for the condenser and reboiler obtained from the short-cut distillation
- Enter the pressure for the Condenser and ensure that you use the correct/right units in which the pressure is being measured
- You may leave the Condenser pressure drop to be 0, unless you know it
- Repeat for the other unit (i.e., Reboiler) and Click NEXT to continue
- The next Screen/Window asks for estimated temperatures for the Condenser and the Reboiler
- These temperatures are taken as initial guesses when HYSYS performs iterations when finding variables
- SKIP the initial guesses and press NEXT
- Specify Reflux Ratio (L/D) (i.e., the value of the External Reflux Ratio) obtained from the short-cut distillation
- Click DONE
- Close window to enable you start entering the feed and other stream conditions
- You may define conditions of each stream by Double Clicking on it, and then Clicking on the DEFINE FROM OTHER STREAM button; this allows you to copy the corresponding stream from the short-cut distillation which you created
- Be careful when you copy to have only the following specifications for the streams
- For the Feed specify two of the following three in the worksheet: Vapor fraction, Temperature and Pressure
- Vapor fraction = 0 means the liquid is at its bubble point
- Vapor fraction = 1 means vapor at its dew point
- Specify BOTH P and T and NO Vapor fraction when the Feed (stream) is a sub-cooled liquid or a superheated vapor
- For the Feed specify either the total Molar or Mass flow rate
- Again, specify either the mole or mass fraction for the Feed
- For the Distillate, double Click on it and ONLY input/specify the Vapor as either 0 = liquid at its bubble point or 1 = vapor at its dew point

- For the Bottoms, double Click on it and again ONLY input/specify the Vapor as either 0 = liquid at its bubble point or 1 = vapor at its dew point
- To Run the A Column Simulation, double click on the Column
- Select MONITOR, and check whether the number of Degrees of Freedom (to the right in the lower corner) is zero (0).
- If the Degrees of Freedom is zero, check the section under specifications, and make sure to activate the independent variables such Reflux Ratio, Bottoms Rate or Distillate Rate which we have selected are checked/activated to enable HYSYS to RUN. In this example, the Reflux Ratio and the Bottoms rate should be checked ratio. The Reflux Rate should be DEACTIVATED (unchecked) since we did not choose it as an independent variable
- Immediately, a value for the Bottoms rate from the short-cut distillation is input following a prompt by HYSYS, the Column Simulator is automatically solved
- A “Converged” icon (green with the word Converged) appears at the bottom indicating that the entire column simulator has been solved
- You can click on Performance, Profiles, Worksheet etc for the results of the Simulation
- To print out your results:
- For streams use: Tools/Workbooks/View and then click File/Print, select All pages and then Print

Dear Dr. Osborne-Lee,

Identify 100
Formulate 100
Solve 50

Total: 250

We are team three (3) writing in response to the Binary Fractional Distillation Column Design assignment. We were given the task of separating 1000 pound mole per hour of a 50-50 homogeneous mixture of ethanol and iso-propanol. The liquid bottom consists of 98 mole percent heavy key and liquid distillate of 99 mole percent light key. Parameters were given in the following terms:

- 1) Feed of saturated liquid at 55 psia.
- 2) Column operation pressure of reflux drum at 18 psia.
- 3) Total condenser used for saturated liquid reflux and liquid distillate.
- 4) Partial reboiler used at the bottom of column for vapor buildup and saturated liquid bottoms.

Within this task theoretical and graphical representations were used in the aid of this design. These included:

- 1) Running a short-cut distillation.
- 2) Modeling a rigorous continuous steady state distillation.
- 3) Construct both a y-x and T-xy diagram by hand and use the McCabe Thiele method to compare to found data

This letter transmits that we have completed these tasks and presents our findings in the following documentation.

Identify
· given ✓
· goal ✓
· sketch ✓
(next, next page)

more goals ✓

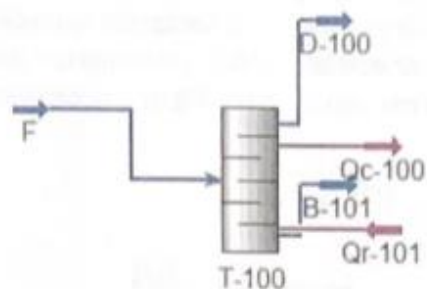
We began by completing the graphical representation of this mixture in a y-x and T-xy diagram. This information allowed us to see the behavior of the components within the mixture. These graphics also helped us to know the theoretical plate number of effective vaporization and condensation steps that were required to achieve a condensate phase at a given composition for the distillate. This process was carried out first by hand using data given and then confirmed using HYSYS, results can be found in the table below.

for mulate

McCabe-Thiele Method	
Bubble Point Temperature of Feed	185 F
Minimum Reflux Ratio	11.19
Minimum Number of Trays	56
Actual Number of Trays	104
Optimal Feed Stage	52
External Reflux Ratio	13.43
Distillate Molar Flow Rate	494.8 lbmol/hr
Bottoms Molar Flow Rate	505.2 lbmol/hr
Condenser Duty	-1.18E8 Btu/hr
Reboiler Duty	1.38E8 Btu/hr
Bubble Point Temperature for Distillate	182.25 F
Bubble Point Temperature for Bottoms	188.9 F
Bubble Point Pressure for Distillate	18 psia
Bubble Point Pressure for Bottoms	18 psia

*104 trays
Separation*

We then did a short-cut distillation simulation, using HYSYS software, that allowed us to find more information on the process. We found that within our column, 130 trays were potentially needed to carry out our distillation process. This large number of trays concurred with our original findings from the McCabe-Thiele method. The results from the simulation are listed in the table below.



Sketch ✓

Figure 1.1: HYSYS Shortcut (1) Diagram

Shortcut Distillation Column 1	
Bubble Point Temperature of Feed	244.1 F
Minimum Reflux Ratio	13.94
Minimum Number of Trays	65
Actual Number of Trays	130
Optimal Feed Stage	75
External Reflux Ratio	16.74
Distillate Molar Flow Rate	494.8 lbmol/hr
Bottoms Molar Flow Rate	505.2 lbmol/hr
Condenser Duty	-1.47E8 Btu/hr
Reboiler Duty	1.45E8 Btu/hr
Bubble Point Temperature for Distillate	182.3 F
Bubble Point Temperature for Bottoms	189.3 F
Bubble Point Pressure for Distillate	18 psia
Bubble Point Pressure for Bottoms	18 psia

A second shortcut distillation was performed increasing the reboiler pressure by 14.14 psia (0.1088 psi drop/tray). The condenser remained at 18 psia, as did the number of trays used in the column, 130. The reflux ratio increased to 17.660 and due to the pressure increase, the temperature of the reboiler increased to 218.6 F. The results are listed in the table below.

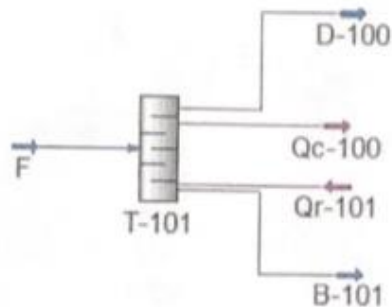


Figure 1.2: HYSYS Shortcut (2) Diagram

Shortcut Distillation Column 2	
Bubble Point Temperature of Feed	244.1 F
Minimum Reflux Ratio	14.71
Minimum Number of Trays	68
Actual Number of Trays	137
Optimal Feed Stage	78
External Reflux Ratio	17.660
Distillate Molar Flow Rate	494.8 lbmol/hr
Bottoms Molar Flow Rate	505.2 lbmol/hr
Condenser Duty	-1.55E8 Btu/hr
Reboiler Duty	1.53E8 Btu/hr
Bubble Point Temperature for Distillate	182.3 F
Bubble Point Temperature for Bottoms	218.6 F
Bubble Point Pressure for Distillate	18 psia
Bubble Point Pressure for Bottoms	32.14 psia

With all simulations and data matching, we were then able to build a model of the continuous steady state distillation process using HYSYS. After numerous trial-and-errors, and assistance from more experienced personnel, we were able to design and run the process within the parameters required.

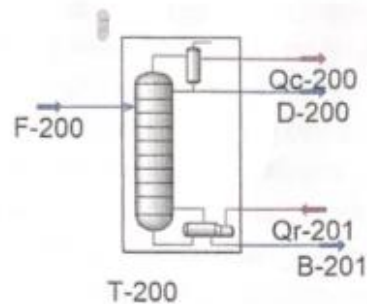


Figure 1.3: Rigorous Distillation Diagram

Rigorous Distillation Column	
Bubble Point Temperature of Feed	244.1 F
Minimum Reflux Ratio	13.94
Minimum Number of Trays	57
Actual Number of Trays	280
Optimal Feed Stage	134
External Reflux Ratio	16.74
Distillate Molar Flow Rate	494.8 lbmol/hr
Bottoms Molar Flow Rate	505.2 lbmol/hr
Condenser Duty	-1.47E8 Btu/hr
Reboiler Duty	1.45E8 Btu/hr
Bubble Point Temperature for Distillate	182.3 F
Bubble Point Temperature for Bottoms	189.3 F
Bubble Point Pressure for Distillate	18 psia
Bubble Point Pressure for Bottoms	18 psia

is this practical?

The decision for the condenser and reboiler pressure to remain the same in the rigorous simulation stems from the comparative results of the two (2) shortcut distillation column simulations. The second shortcut distillation column, where the reboiler pressure was increased to 32.14 psia, yields a similar result of actual trays needed to that of the first shortcut distillation column. Since increasing pressure would increase the cost of the initial process, the option to remain at constant pressure was used. The rigorous distillation column has a high number of stages due to the composition factor of both the light and heavy key component. The simulation was tried at 130 stages. The results of this run, x_L in the distillate was 0.9677 and x_H in the distillate was 0.0323. The corresponding values in the bottoms were 0.0418 and 0.9582. To obtain a closer composition factor we then tried 200 stages. The x_L in the distillate was 0.9823 and the x_H in the distillate was 0.0177. The x_H in the bottoms was 0.9725 and the x_L in the bottoms was 0.0275. After several trial-and-error runs, we reached a stage number of 280. We believe this number is high due to the similar boiling points of ethanol and iso-propanol. The separation of these analogous liquids result in many stages to achieve such a high molar composition in both the distillate and the bottoms stream.

Software reports along with the T-xy diagram and y-x diagram can be found below in the attachments to provide visual aid regarding our results.

Sincerely,

Team 3

Kayla Albus

Khristen Liverman

Danria Taylor

Good work
team 3!

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PRAIRIE VIEW A M UNIVERS

Bedford, MA

USA

Case Name:Shortcut.hsc

Unit Set:Field

Date/Time:Wed May 06 14:07:45 2020

Workbook: Case (Main)

Material Streams

Fluid Pkg:All

Name	F	D-100	B-101		
Vapour Fraction	0.0000 *	0.0000	0.0000		
Temperature (F)	244.1	182.3	189.3		
Pressure (psia)	55.00 *	18.00	18.00		
Molar Flow (lbmole/hr)	1000 *	494.8	505.2		
Mass Flow (lb/hr)	5.308e+004	2.287e+004	3.022e+004		
Liquid Volume Flow (barrel/day)	4603	1967	2635		
Heat Flow (Btu/hr)	-1.212e+008	-5.756e+007	-6.632e+007		

Compositions

Fluid Pkg:All

Name	F	D-100	B-101		
Comp Mole Frac (Ethanol)	0.5000 *	0.9900	0.0200		
Comp Mole Frac (2-Propanol)	0.5000 *	0.0100	0.9800		

Energy Streams

Fluid Pkg:All

Name	Qc-100	Qr-101			
Heat Flow (Btu/hr)	-1.474e+008	1.448e+008			

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
T-100	Shortcut Column	F	D-100	No	500.0 *
		Qr-101	B-101		
			Qc-100		

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Page 1 of 1

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* Specified by user

1	 PRAIRIE VIEW A M UNIVERS Bedford, MA USA		Case Name: Shortcut2.hsc			
2			Unit Set: Field			
3			Date/Time: Wed May 06 14:57:42 2020			
4						
5						
6	Workbook: Case (Main)					
7						
8						
9	Material Streams Fluid Pkg: All					
10						
11	Name	F	D-100	B-101		
12	Vapour Fraction	0.0000 *	0.0000	0.0000		
13	Temperature (F)	244.1	182.3	218.6		
14	Pressure (psia)	55.00 *	18.00	32.14		
15	Molar Flow (lbmole/hr)	1000 *	494.8	505.2		
16	Mass Flow (lb/hr)	5.308e+004	2.287e+004	3.022e+004		
17	Liquid Volume Flow (barrel/day)	4603	1967	2635		
18	Heat Flow (Btu/hr)	-1.212e+008	-5.756e+007	-6.558e+007		
19						
20	Compositions Fluid Pkg: All					
21	Name	F	D-100	B-101		
22	Comp Mole Frac (Ethanol)	0.5000 *	0.9900	0.0200		
23	Comp Mole Frac (2-Propanol)	0.5000 *	0.0100	0.9800		
24						
25	Energy Streams Fluid Pkg: All					
26	Name	Qc-100	Qr-101			
27	Heat Flow (Btu/hr)	-1.551e+008	1.531e+008			
28						
29	Unit Ops					
30	Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
31	T-101	Shortcut Column	F	D-100	No	500.0 *
32			Qr-101	B-101		
33				Qc-100		
34						
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63	Aspen Technology Inc.		Aspen HYSYS Version 9		Page 1 of 1	

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aspentech

PRAIRIE VIEW A M UNIVERS

Bedford, MA

USA

Case Name:

Rigorous.hsc

Unit Set:

Field

Date/Time:

Wed May 06 14:00:56 2020

Workbook: T-200 (COL1)

Material Streams

Fluid Pkg: All

Name	Reflux	To Condenser	Boilup	To Reboiler	D-200
Vapour Fraction	0.0000	1.0000	1.0000	0.0000	0.0000
Temperature (F)	182.3	182.3	189.3	189.3	182.3
Pressure (psia)	18.00	18.00	18.00	18.00	18.00
Molar Flow (lbmole/hr)	8284	8779	8565	9070	494.8
Mass Flow (lb/hr)	3.828e+005	4.057e+005	5.118e+005	5.420e+005	2.287e+004
Liquid Volume Flow (barrel/day)	3.294e+004	3.490e+004	4.463e+004	4.726e+004	1967
Heat Flow (Btu/hr)	-9.635e+008	-8.736e+008	-9.791e+008	-1.190e+009	-5.756e+007
Name	B-201	F-200			
Vapour Fraction	0.0000	0.0000			
Temperature (F)	189.3	244.1			
Pressure (psia)	18.00	55.00			
Molar Flow (lbmole/hr)	505.2	1000			
Mass Flow (lb/hr)	3.022e+004	5.308e+004			
Liquid Volume Flow (barrel/day)	2635	4603			
Heat Flow (Btu/hr)	-6.632e+007	-1.212e+008			

Compositions

Fluid Pkg: All

Name	Reflux	To Condenser	Boilup	To Reboiler	D-200
Comp Mole Frac (Ethanol)	0.9900	0.9900	0.0246	0.0244	0.9900
Comp Mole Frac (2-Propanol)	0.0100	0.0100	0.9754	0.9756	0.0100
Name	B-201	F-200			
Comp Mole Frac (Ethanol)	0.0200	0.5000			
Comp Mole Frac (2-Propanol)	0.9800	0.5000			

Energy Streams

Fluid Pkg: All

Name	Qc-200	Qr-201			
Heat Flow (Btu/hr)	1.474e+008	1.447e+008			

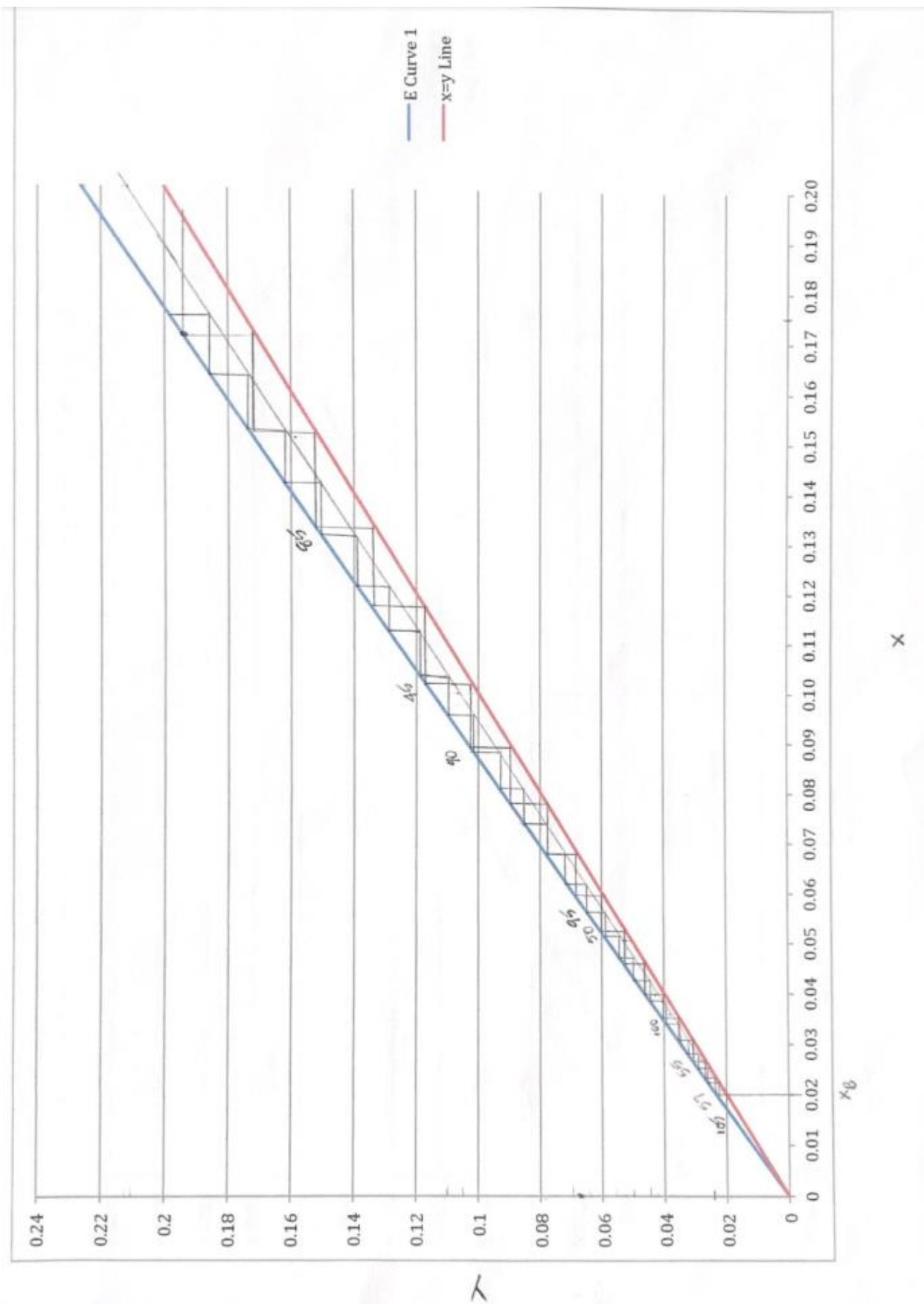
Unit Ops

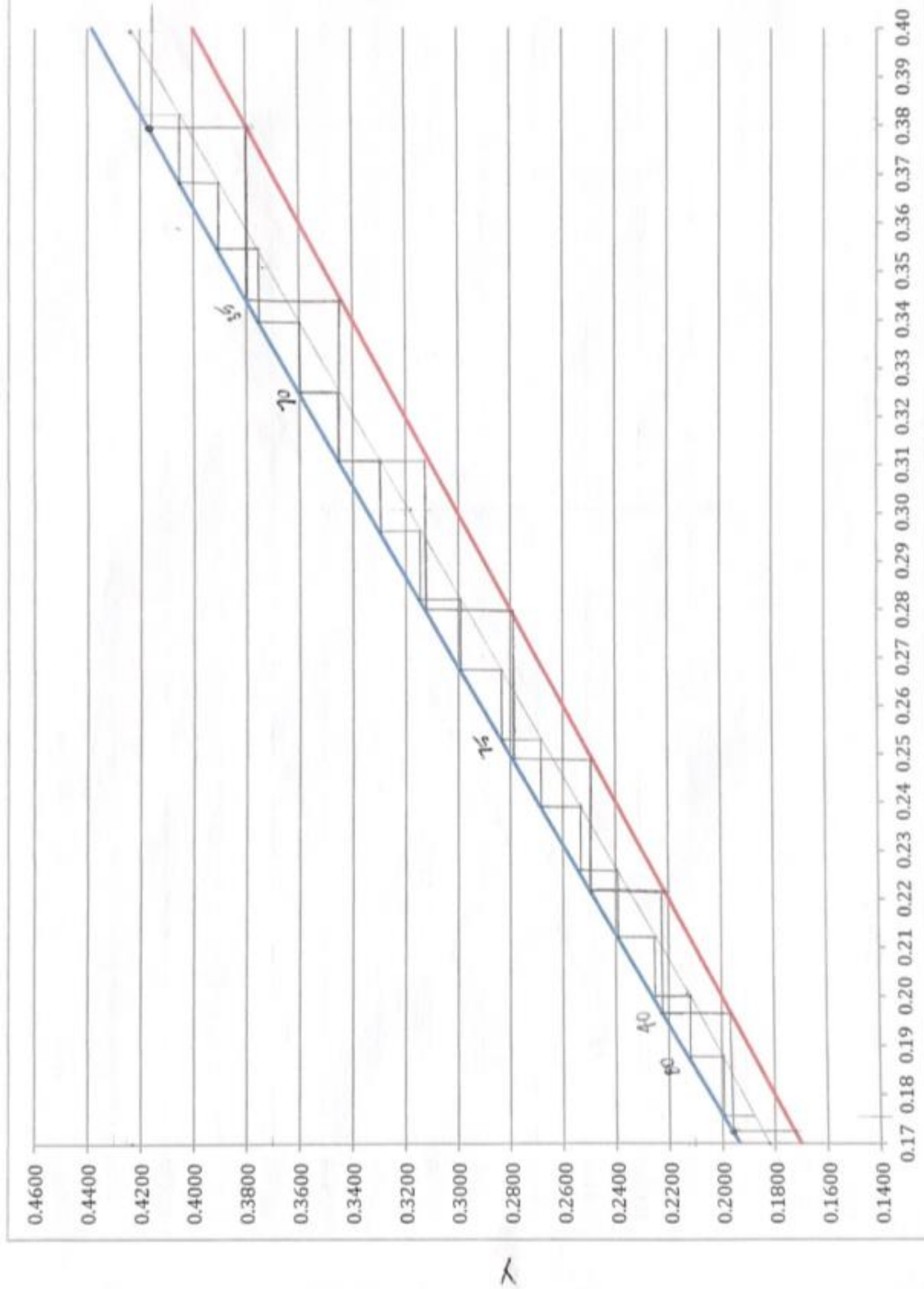
Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
Reboiler	Reboiler	To Reboiler	B-201	No	500.0 *
		Qr-201	Boilup		
Main Tower	Tower	Reflux	To Reboiler	No	500.0 *
		Boilup	To Condenser		
		F-200			
Condenser	Total Condenser	To Condenser	D-200	No	500.0 *
		Qc-200	Reflux		
			Qc-200		

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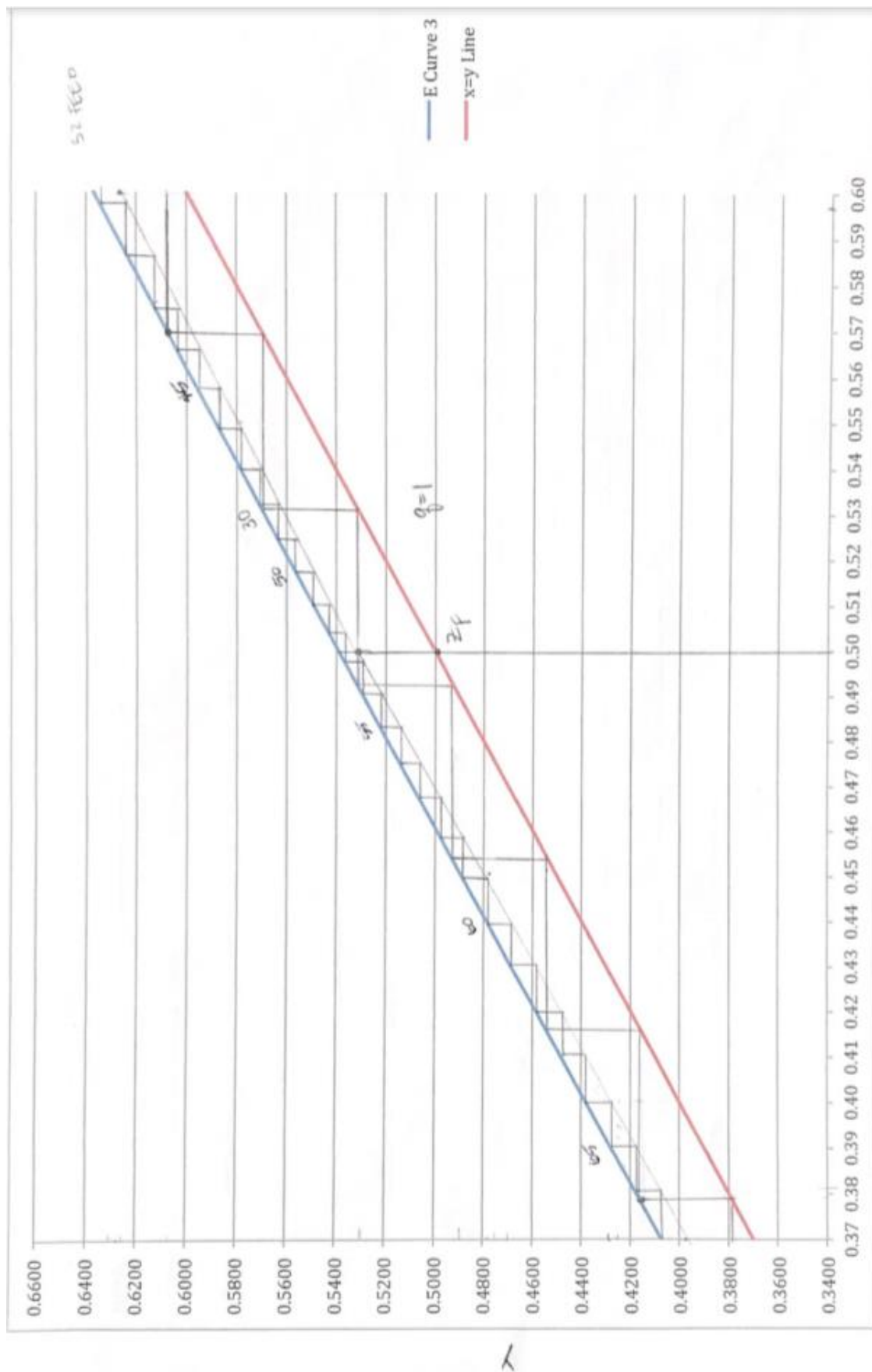
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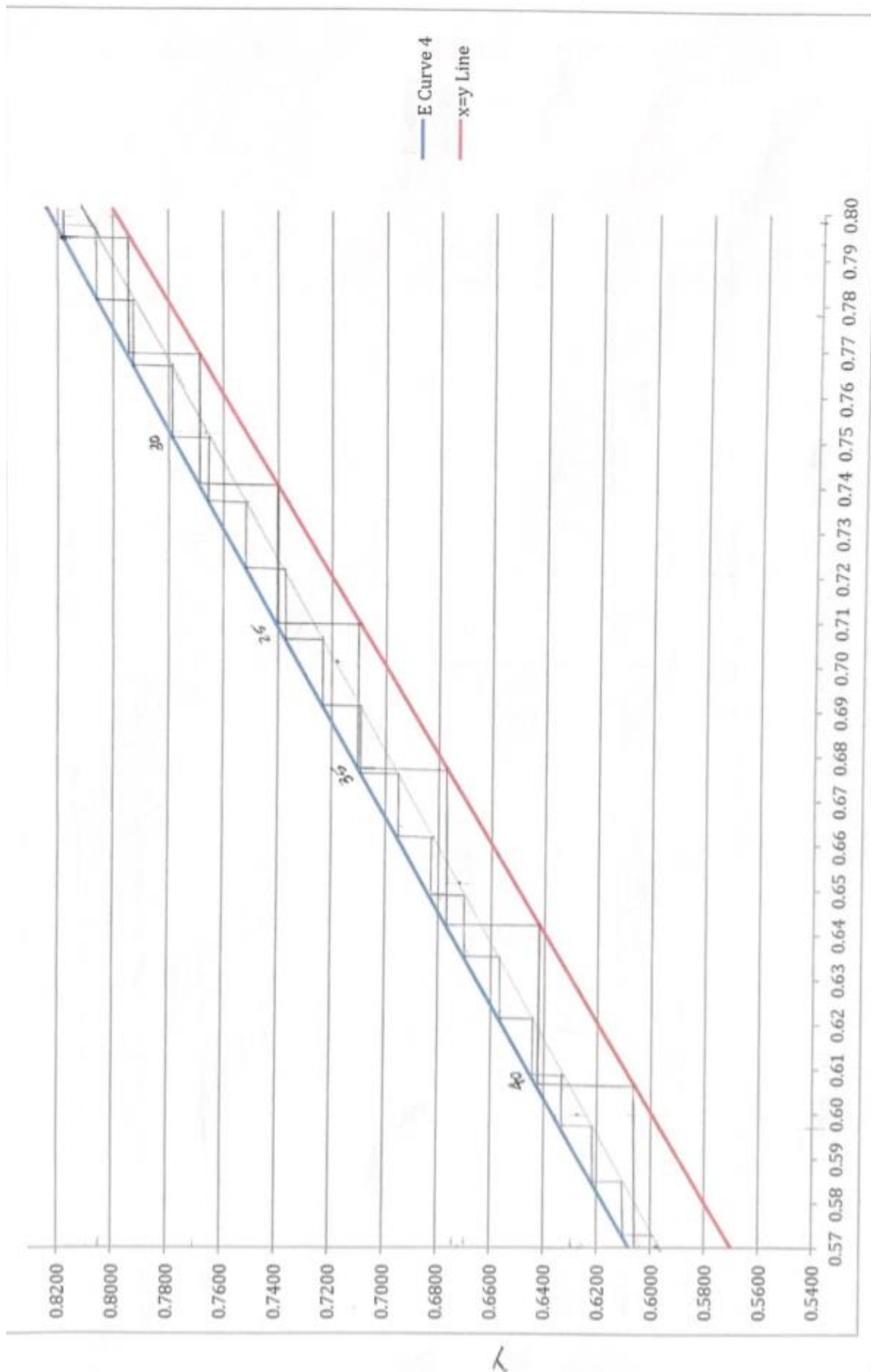


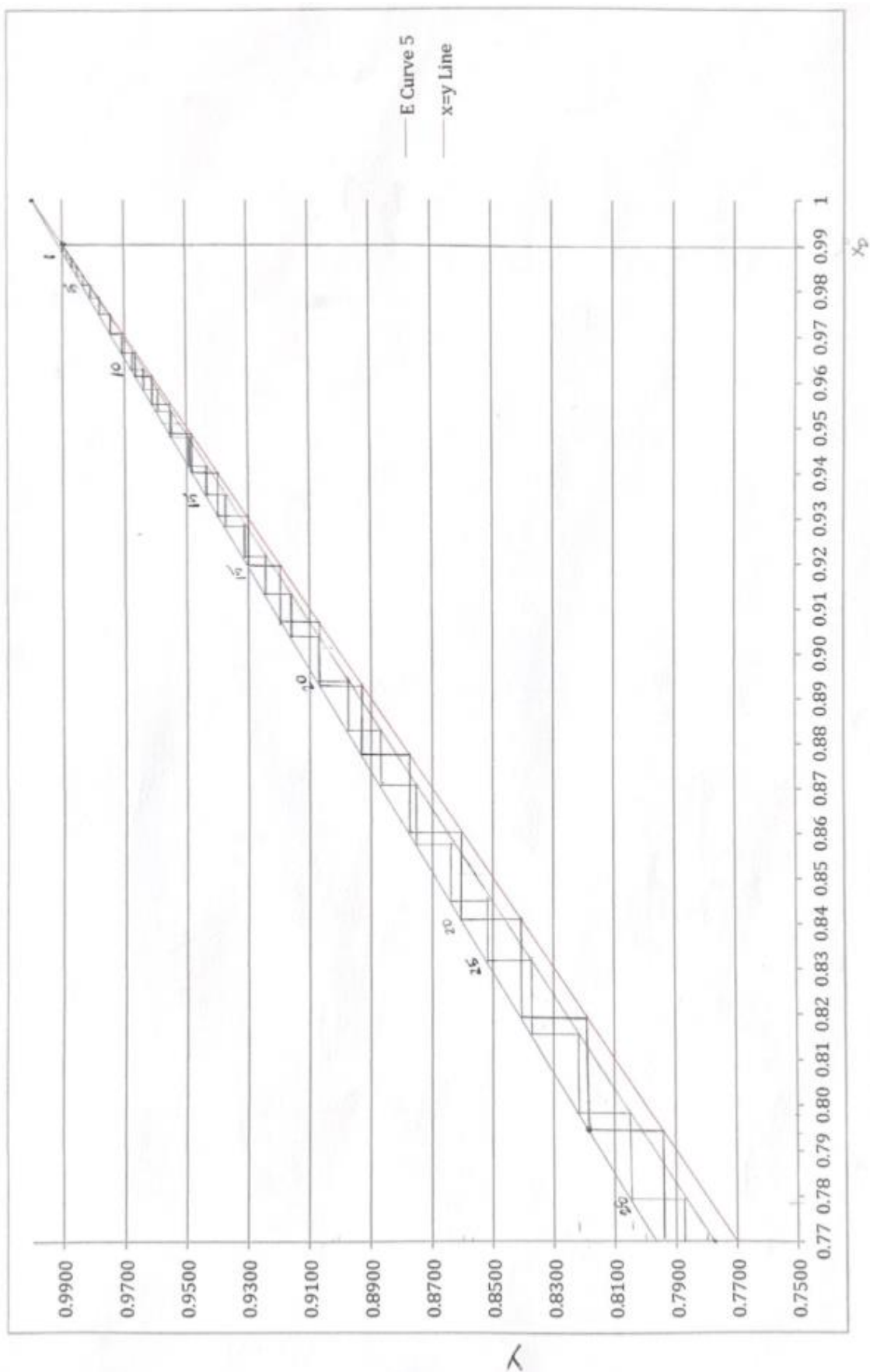


x

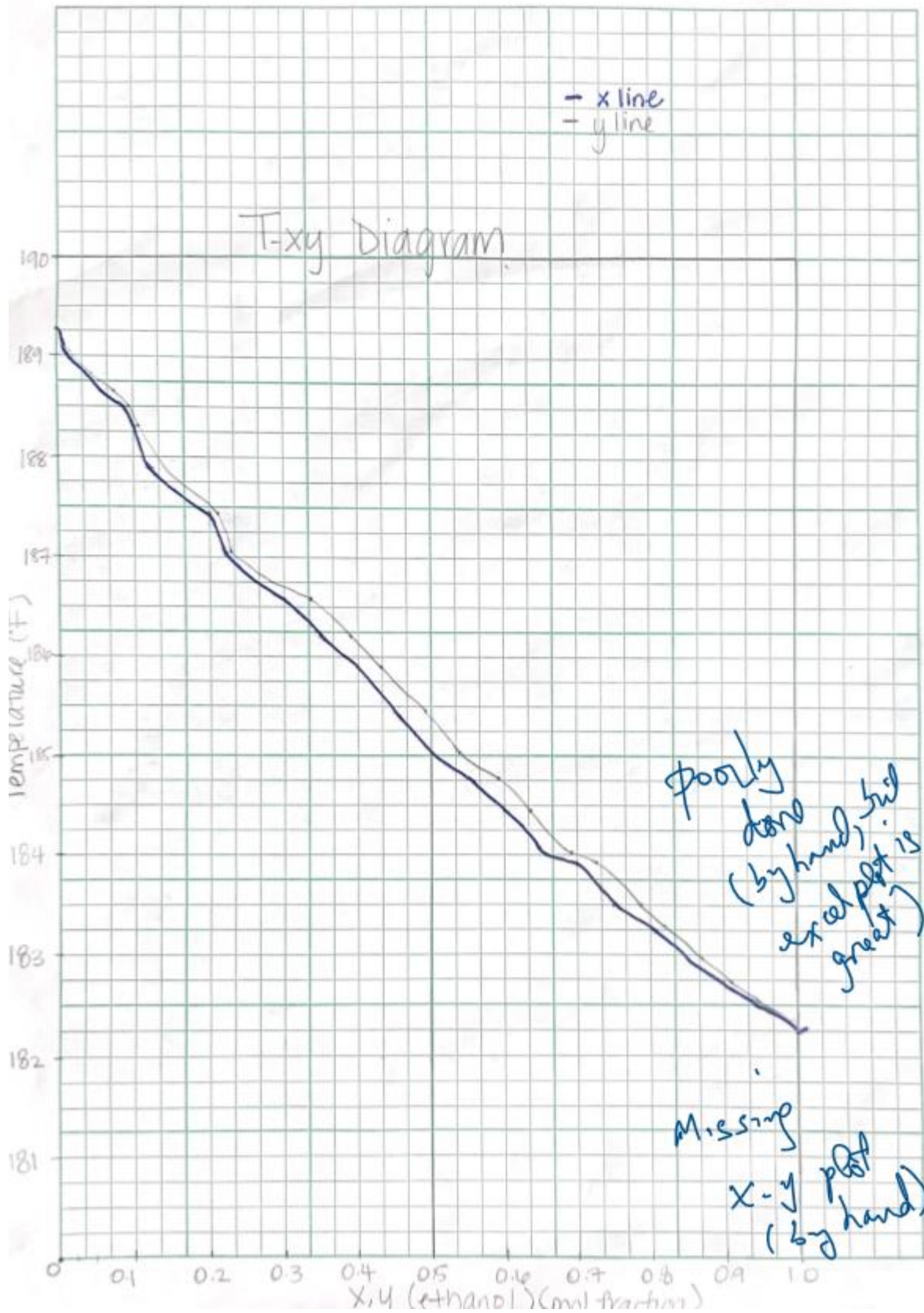


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**OUTCOME SPECIFIC ASSIGNMENTS
USED TO ASSESS OUTCOMES**

ASSIGNMENTS FOR OUTCOME 1

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

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET**

Process Control

FALL 2021

Instructor: Dr. Jorge F. Gabitto

Title of Assignment

Homework 3

Outcome Measured Using this Assignment

Outcome 1

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

Brief justification of why this assignment is suitable for this outcome

The rubric used for grading this assignment measures the students' ability to identify, solve, and formulate engineering problems. It applies Laplace domain analysis of transient behavior of complex systems.

CHEG 4033
3rd HomeWork

1). Calculate the Laplace equivalent of the following equations:

- A step of size Du
- A pulse of integral P
- $\sin(\omega t)$
- $\frac{dT}{dt} = K_p u$

2). Calculate the Laplace equivalent of the following equations:

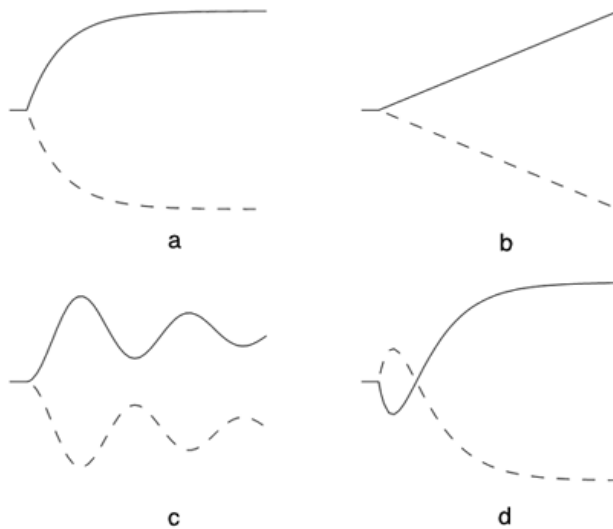
$$\tau_p \frac{dT}{dt} = (u_1 - T) + u_2 A + u_3 B,$$

where T is the output variable, A and B are constants and u_1 , u_2 and u_3 are the deviations variables for the input temperature (Ti), input flow (Fi) and input heat flow (QF), respectively.

$$\tau_p \frac{d^2T}{dt^2} + \frac{dT}{dt} A = (u_1 - T) + u_2 B + \frac{du_3}{dt},$$

where T is the output variable, A, B, and C are constants and u_1 , u_2 and u_3 are the deviations variables for the input temperature (Ti), input flow (Fi) and input heat flow (QF), respectively.

3). Describe qualitatively the following dynamic responses to a step in the input variable:



Hint: Analyze response at short times, functional description, and convergence of the eight systems shown above, 4 given by solid lines and 4 given by broken lines.

1ke

$$2. T_p \frac{dT}{ds} = (u_1 - \bar{T}) + u_2 A + u_3 B$$

$$L(T_p \frac{dT}{ds}) = L((u_1 - \bar{T}) + u_2 A + u_3 B)$$

$$T_p sT(s) - T(0) = T_1(s) - \bar{T}(s) + A F_i(s) + B Q_F(s)$$

$$T(0) + T_p sT(s) - T_1(s) + A F_i(s) + B Q_F(s)$$

$$T(0) (1 + T_p s) T_i(s) + A F_i(s) + B Q_F(s)$$

$$T(0) = \frac{T_1(s) + A F_i(s) + B Q_F(s)}{1 + T_p(s)}$$

Ike Anaghara

3.

a) Solid - Direct, monotonic, convergent
Dotted - Reverse, monotonic convergent

b) Solid - Direct, monotonic, convergent
Dotted - Reverse, monotonic, convergent

c) Solid - Direct, oscillatory, convergent
Dotted - Reverse, oscillatory, convergent

d) Solid - Reverse π , monotonic, converge
Dotted - Reverse π , monotonic, converge

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1

• A step of size D_u : $\mathcal{L}[D_u] = \frac{D_u}{s}$

• A pulse of integral: $\mathcal{L}\left[\int_0^t P dt\right] = \frac{P}{s^2}$

• $\sin(\omega t)$: $\mathcal{L}[\sin(\omega t)] = \frac{\omega}{s^2 + \omega^2}$

• $\frac{dT}{dt} = k_p U$: $\mathcal{L}\left[\frac{dT}{dt}\right] = \mathcal{L}[k_p U]$

$$sT(s) = k_p U(s)$$

WATCH

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET**

Process Control

FALL 2021

Instructor: Dr. Jorge F. Gabitto

Title of Assignment

Test 3

Outcome Measured Using this Assignment

Outcome 1

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

Brief justification of why this assignment is suitable for this outcome

The rubric used for grading this assignment measures the students' ability to identify, solve, and formulate engineering problems. It applies Laplace domain analysis and algebraic manipulations to determination of transient behavior of complex systems.

CHEG 4303
Process Control
3rd Exam A

1). Calculate for the simplified two block (process and controller) block diagram the response to a negative step change ($-2/s$) if the controller is a PI. Calculate the long term value. Plot the response.

Use: $G_{ca}(s) = (0.5/s + 1)$, $G_{sys}(s) = 2 / (5s + 1)$.

2). Calculate the qualitative behavior of a closed control loop that has the following roots:

Zeros (top): $z_1 = -0.5$, $z_2 = -0.2$,

Poles (bottom): $p_1 = -1$, p_2 and p_3 are complex numbers with **real part** = -2 and imaginary parts = 3 and -3 , respectively. Justify and plot the response.

$$(1) G_{total} = \frac{G_{CA} G_{sys}}{1 + G_{CA} G_{sys}}$$

Calculate for simple
2 block diagram
- response
- long term value

$$G_{CA} = (1/s + 0.5s + 1) \quad \text{--- } (K_P)$$

$$G_{sys} = 2 / (s + 1) \quad \text{or}$$

$$\frac{2}{(s + 1)} \quad \begin{matrix} \text{--- } (K_{sys}) \\ \text{--- } (T_{sys}) \end{matrix}$$

a) Dynamiz Behavior
- closed control loop
- use G_{total}

$$1) G_{CA} \times G_{sys} = (1/s + 0.5s + 1) \times \left(\frac{2}{(s + 1)} \right)$$

$$= \frac{\frac{2}{s} + 1s + 2}{(s + 1)}$$

$$G_{Total} = \frac{\frac{2}{s} + 1s + 2}{s + 1}$$

$$\frac{(s + 1)}{(s + 1)} \times 1 + \frac{\frac{2}{s} + 1s + 2}{s + 1}$$

$$\frac{\frac{2}{s} + 1s + 2}{s + 1}$$

$$\frac{s + 1 + \frac{2}{s} + 1s + 2}{s + 1} \quad [G_{Total}]$$

$$= \frac{\frac{2}{s} + 1s + 2}{s + 1 + \frac{2}{s} + 1s + 2}$$

$$= \left[\frac{\frac{2}{s} + 1s + 2}{6s + \frac{2}{s} + 3} \right]$$

a) Direct / Reverse

Dynamic response

$$G_{CA} = (1/s + 0.5s + 1) \rightarrow \text{Direct}$$

- Constant; no root
- positive

b) real root

$$\text{Denominator} = 5s + 1 = 0$$

$$\frac{5s}{5} = \frac{-1}{5}$$

$$s = -1/5$$

real root

= monotonic
or
Non-oscillatory

c) convergent + Divergent

$$s < 0 \text{ (All)} \Rightarrow \text{convergent (Stable)}$$

Plot

Direct, monotonic, Convergence



values? Long term + Short Term

$$U(s) = \frac{1}{s} \text{ (Step of value)}$$

$$= s \times G_{\text{total}} \times \overline{U}(s) =$$

$$= \cancel{s} \times \left[\frac{\frac{2}{s} + 1s + 2}{6s + \frac{2}{s} + 3} \right] \times \frac{1}{\cancel{s}} = \boxed{\frac{\frac{2}{s} + 1s + 2}{6s + \frac{2}{s} + 3}}$$

$$\begin{array}{l} \text{long term lim} \\ s \rightarrow 0 \\ s=0 \end{array} \quad \frac{\cancel{\frac{2}{s}} + \cancel{1s} + 2}{\cancel{6s} + \cancel{\frac{2}{s}} + 3} = \boxed{\frac{2}{3}} \text{ long term value} \quad \checkmark$$

Jarred Essilima

Exam 3-E

2 Calculate the qualitative behavior of closed loop:

(a) short-term Behavior

Top: $z_1 = -0.5$, $z_2 = 0.2$

bottom: $p_1 = -1$

Reverse

$p_2 = (-2, 3)$

$p_3 = (-2, -3)$

real
imaginary

(b) Oscillatory $\begin{pmatrix} -2 \\ -2 \end{pmatrix}$ Functional Behavior of the output response.

(c) $-2 < 0 \Rightarrow$ Convergent Long-term Behavior

Plot

