

**PRAIRIE VIEW A&M UNIVERSITY
ROY G. PERRY COLLEGE OF ENGINEERING
DEPARTMENT OF CHEMICAL ENGINEERING
CHEG 3304 Chemical Engineering Thermodynamics II
SPRING 2022**

I. COURSE DESCRIPTION IN ABET FORMAT

II STUDENT PERFORMANCE ASSESSMENT

Course Outcomes Taught (None Assessed)

Summary of Student Performance

End of Course Observations

II. PROJECT WRITTEN REPORTS

Summary of Topics covered by Test

Original Test Questions & Master Solution/grading scheme used

(Summary of topics can be a separate page or include on the assignment itself)

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

III. PROJECT ORAL REPORTS (VIDEO ARTICULATION)

Summary of Topics covered by Test

Original Test Questions & Master Solution/grading scheme used

(Summary of topics can be a separate page or include on the assignment itself)

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

III. QUIZZES

Summary of Topics covered by Quiz

Original Quiz Questions & Master Solution/grading scheme used

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

IV. EXERCISES

Summary of Topics covered by Homework

Original Homework Questions & Master Solution/grading scheme used

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

V. DISCUSSION FORUM POSTS

List of topics covered by forum

Discussion Forum Instructions and Grading Scheme

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

Course Description in ABET Format

CHEMICAL ENGINEERING DEPARTMENT CHEG 3304 CHEMICAL ENGINEERING THERMODYNAMICS II

1.	Course number and name:	CHEG 3304 Chemical Engineering Thermodynamics II
2.	Credits and contact hours:	3 credit hours; 3 contact hours
3.	Instructor's or course coordinator's name:	Dr. Ernest Carl McIntyre, Adjunct Professor of Chemical Engineering
4.	Text book: Title:	Introduction to Chemical Engineering Thermodynamics
	Author:	J. M. Smith, H. C. Van Ness, and M. M. Abbott
	Publisher, Year & Edition:	7th edition, McGraw-Hill, 2001, ISBN: 0-07-310445-0 (preferred); or more recent edition. Authors website: http://www.mhhe.com/engcs/chemical/smith/
	a. Other Supplemental material	1. LearnChemE.com (last accessed 1/18/2021) http://www.learncheme.com/ . In particular, many of the screencasts on thermodynamics, http://www.learncheme.com/screencasts/thermodynamics 2. Devoe (last accessed 1/18/2021) http://www2.chem.umd.edu/thermobook/ , open source textbook.
5.	Specific course information	
	a. Brief description of the content of the course (catalog description)	Credit 3 semester hours. Properties of ideal and non-ideal binary and multi-component mixtures. Studies of equilibrium for single-and multi-component systems based on methods of corresponding states, equations of state and activity coefficients. Chemical equilibrium applied to both homogeneous and heterogeneous systems.
	b. Prerequisites or Co-requisites	CHEG 2334 (2043) and MATH 2320 (2043)
	c. *Indicate whether a required, elective, or selected elective (as per definition provided) course in the program	Required
6.	a. Specific goals for the course specific outcomes of instruction (e.g. The student will be able to explain the significance of current research about a particular topic.) <i>Students will be able to :</i>	b. Explicitly indicate which of the student outcomes listed in Criterion 3 or any other outcomes are addressed by the course. <i>The specific goals for the course specific outcomes listed on the left column will address the following student learning outcomes:</i>
	1. Demonstrate knowledge of the 1st, 2nd and 3rd laws of thermodynamics	Outcome 1 An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.
	2. Apply knowledge of 1st and 2nd laws of thermodynamics to identify, formulate and solve problems in energy conservation, power cycles, refrigeration cycles and liquefaction systems	

	3. Apply knowledge of multi-component mixture physical equilibrium, and chemical equilibrium to identify, formulate and solve problems in reacting and non-reacting systems		
	4. Demonstrate use of modern tools of the profession in solving multi-component mixture physical equilibrium problems in reacting and/or non-reacting systems		
7	Brief list of topics to be covered	Review 1 st , 2 nd & 3 rd laws (chapters 1-5) (6 hours) Ideal gas law (3 hours) Thermodynamic properties of fluids: states of matter, energy & entropy changes (6 hours) Maxwell's relations, equations of state, property relationships (3 hours) Residual properties (4 hours) Power & refrigeration cycles (6 hours) Vapor/liquid equilibrium (6 hours) Solution thermodynamics (6 Hours) Gamma Phi Formulation (3 hours) Project activities (3 hours) Total (45 hours)	



II STUDENT PERFORMANCE ASSESSMENT

Program Outcomes Assessed in this course: None

Program Outcomes Developed in this course: One outcome as shown below.

Outcome 1:

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

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Assessment Summary of Class Semester Averages for Outcomes

Not applicable

Student Performance Summary (Class Averages by Assignment Category)

Gradebook Summary

CHEMICAL ENGINEERING THERMODYNAMICS II SPRING 2022

**Title of Assignment: UPLOAD LETTER REPORT FOR PROJECT 1
Refrigeration Cycle Design Project**

TOPICS COVERED IN PROJECT 1

Project 1 covered the following topics:

1. Review of the 1st and 2nd laws of thermodynamics
2. Introduction of refrigeration cycle with application of thermodynamic principles
 - a. Cycles and state properties
 - b. Isothermal, isobaric, reversible, and irreversible processes
 - c. Use of thermodynamic tables
 - d. Real vs. ideal gas behavior
3. Concept of efficiency: compressor efficiency, cycle efficiency and coefficient of performance
4. Phase diagrams (p-H and T-S diagrams) and their use in representing and analyzing a refrigeration cycle
5. Application of 2nd law and concept of approach temperature in selecting condenser & evaporator operating pressure
6. Refrigerant selection based on operating pressure/temperature and global warming potential (GWP)
7. Experience working in teams
8. Written communication

**CHEMICAL ENGINEERING THERMODYNAMICS II
SPRING 2022**

**SAMPLE PROJECT REPORTS
AND GRADING RUBRIC FOR PROJECT 1**

ABOVE AVERAGE

REFRIGERATION CYCLE DESIGN LETTER REPORT

Date: March 4, 2022
To: Professor McIntyre
From: Laury Mengue, Ruel Wright
Re: Project #1 Design of a Refrigeration cycle

INTRODUCTION

Refrigeration cycles are conceptual and mathematical models for heat pumps, air conditioning and refrigeration systems. The purpose of a refrigeration system is to transmit heat from one location at a higher temperature to another location at a higher temperature.

PROBLEM STATEMENT

A refrigeration system is to be designed to maintain the temperature in the range T_{LOWmin} to T_{LOWmax} , while the outside temperature varies from $T_{HIGHmin}$ to $T_{HIGHmax}$, as given in the team assignment matrix below. The total thermal load on the storage unit is given as 36 kW. Obtain an initial design for the vapor compression refrigeration system shown in Figure 1. Choose a safe and suitable refrigerant. For safe operation and other factors, such as additional energy transfer, design the system using a safety factor of 1.25. The compressor efficiency could range from 60 to 80 percent.

In the course of your design you will need to specify or/and determine the temperatures and pressures at the different states and show the cycle with the vapor dome on a temperature entropy (T-s) diagram or pressure enthalpy (p-h) diagram, or both. Also, you must determine the coefficient of performance value and the mass flow rate of the working fluid.

OBJECTIVE

There were 4 major focal points for this project:

- Design of the refrigeration system to maintain the following temperature ranges. $T_{Low}(min) = -20^{\circ}C$, $T_{Low}(max) = -10^{\circ}C$, $T_{High}(min) = 15^{\circ}C$ and $T_{High}(max) = 25^{\circ}C$ and talk about its components and its process.
- Choose a refrigerant with a safety factor of 1.25 and a compressor efficiency that ranges from 60-80% and show the formulas that will be used for our calculations.
- Determine the temperatures and pressures at the different states and show the cycle vapor dome on a T-S diagram or a P-H diagram.

- Determine the coefficient of Performance (cop) value and the mass flow rate of the working fluid.

DESIGN METHODOLOGY

Refrigeration process

A refrigeration cycle has 4 major components:

- Compressor: Its purpose is to circulate the refrigerant in the system. The refrigerant is compressed from a cool gaseous state to a hot high pressure vapor. Then, the refrigerant moves to the condenser.
- Condenser: Its purpose is to change the hot gas into a liquid. The condenser does so by allowing the high pressure and decrease in temperature to condense the vapor which ejects heat.
- Thermal Expansion Valve: Its main purpose is to provide an environment that allows for the refrigerant to decrease in pressure.
- Evaporator: The purpose of the refrigerant is to remove heat which allows for the refrigerant to cool down. Inside the evaporator, the liquid refrigerant is expanded and evaporated.

Assumptions

For the purpose of this project, assumptions need to be made in order to facilitate the calculations:

- The four components operate under steady-state, steady-flow process.
- Both the compressor and the expansion device are considered adiabatic
- Enthalpy $H_3 = H_4$
- Pressure $P_3 = \text{Pressure } P_2$
- Efficiency used = 70%

Procedure and Formulas

For the effectiveness of our design, we utilized a vapor compression refrigeration cycle. Also, we applied the first and second Laws of Thermodynamics while taking in consideration the assumptions mentioned above. See below in table 1, the formulas used:

Table 1

Compressor: Work done in the compressor	$W_{in} = m(H_2 - H_1)$
Condenser: Heat released out of the system by the condenser	$Q_{out} = m(H_3 - H_2)$

Throttle (Expansion Valve): $H_3 - H_4$	$dS = 0$, $W_{net} = 0$ and $Q_{net} = 0$
Evaporator : Heat entering the evaporator	$Q_{in} = \dot{m}(H_1 - H_4)$
Coefficient of Performance(COP)	$COP = \frac{Q_{in}}{W_{in}}$
Isentropic Entropy	$\eta_c = \frac{W_{ideal}}{W_{actual}} \times 100\%$
Linear Interpolation	$y = y_1 + (x - x_1)((y_2 - y_1)/(x_2 - x_1))$

W_{in} = Power entering the compressor
 $\dot{m}$ = Mass flow rate of the refrigerant
 Q_{in} = Heat absorbed by the evaporator
 Q_{out} = Heat ejected by the condenser
 H = Enthalpy

After stating the formulas utilized for our Project, we are going to select our refrigerant.

Refrigerant selection

After considering many refrigerants , we chose R-134A also known as 1,1,1,2-Tetrafluoroethane because it's safe for the environment, easily accessible, It's not highly flammable, safe for humans and convenient to operate at our temperatures.

For the purpose of our project, we will operate within the following given temperatures : T-Low (min) = -20°C , T-Low(max) = -10°C, T-High(min) = 15°C and T-High(max) = 25°C. We also assume an Isentropic efficiency of 70% and our refrigerant has a safety factor of 1.25.

The third objective is to show the refrigeration schematic diagram with values for P (Pressure), T (Temperature), H (Enthalpy), S (Entropy) and V (Volumetric Density)at each stage. We will be using the Properties of Saturated table for R-134A and The P-H diagram.

See below Figure 1 representing a schematic diagram of the refrigeration cycle. It shows the major components, the different states(Vapor and/or Liquid), the direction of the refrigerant and Pressure and temperature at different stages.It is also important to underline that we used Linear Interpolation to calculate these values.

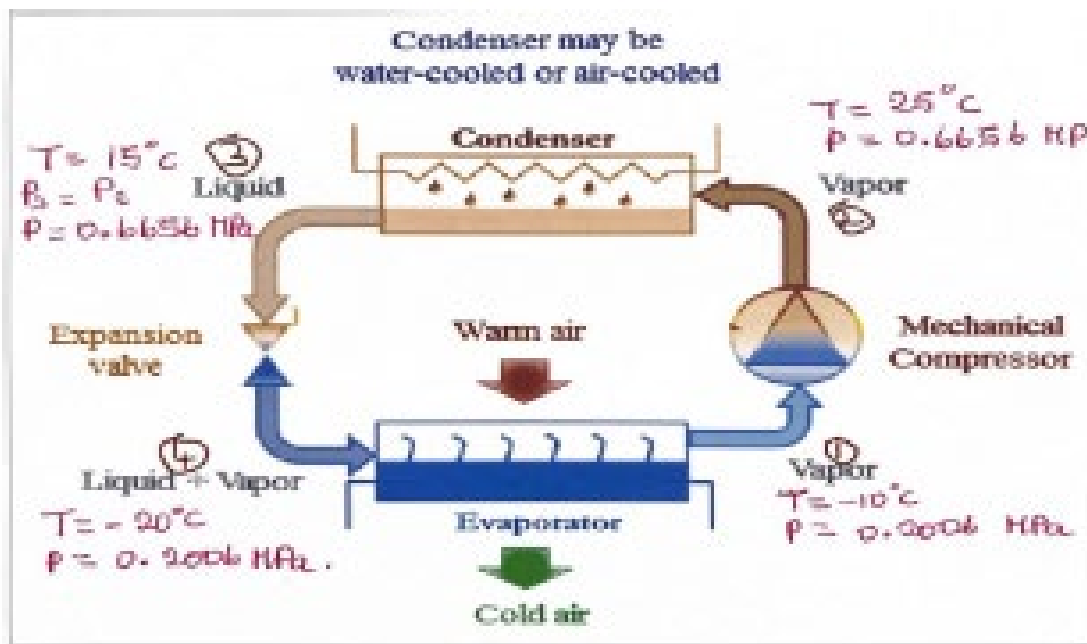


Figure 1: Diagram of Vapor Compression Refrigeration Cycle

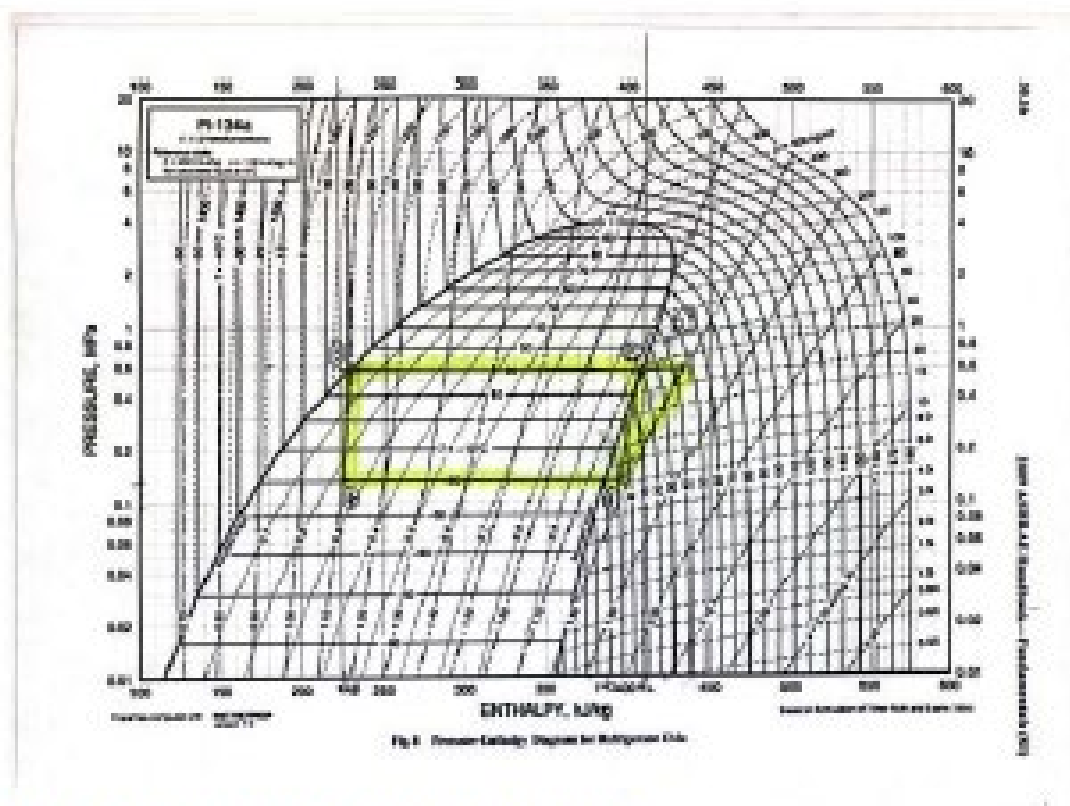


Figure 2: Pressure Enthalpy Diagram For R-134A

RESULTS

As previously mentioned above the values for T, P, H, V and S were obtained from the P-H Diagram and the Properties of Saturated table for R-134A from PVAMU Canvas course Modules. See below a summary of these values at different stages.

	Stage 1	Stage 2	Stage 2'	Stage 3	Stage 4
T (°C)	-10	25	41	15	-20
P (MPa)	0.2006	0.6656	0.6656	0.6656	0.1327
H (KJ / Kg)	392.66	412.33	430.85	220.48	220.48
S (KJ/ Kg.K)	1.7334	1.7334	1.7812	1.0724	0.9002
V (m ³ / Kg)	0.0996	0.03043	0.0396	0.0421	0.14739

Finally, we have to calculate the Coefficient of Performance and the Mass flow rate of our refrigerant.

Calculation of COP

$$COP = \frac{Q_{in}}{W_{in}} = \frac{\dot{m}(H1 - H4)}{\dot{m}(H2' - H1)} = \frac{H1 - H4}{H2' - H1} = \frac{392.66 - 220.48}{430.85 - 392.66} = 4.5$$

Calculation of mass flow rate $\dot{m}$

We know : $Q_{in} = \dot{m}(H1 - H4)$, Therefore

$$\dot{m} = \frac{Q_{in}}{H1 - H4} = \frac{36 \text{ kW}}{392.66 - 220.48} = 0.204 \text{ Kg / s}$$

DISCUSSION

Figure 1 shows the refrigeration cycle and the states with the corresponding temperatures and pressure.

Figure 2 shows a pressure-enthalpy diagram for R-134a. Based on the diagram, the refrigerant is a saturated vapor at state 1, a superheated gas at state 2, a liquid at state 3, and a liquid-gas mixture at state 4.

Table 1 shows the different components in a refrigeration cycle and their respective equations.

At state 1, the fluid is at a temperature of -10°C as it comes out the evaporator as a saturated vapor; with a pressure of 0.20060 mpa, enthalpy of 392.67 KJ/Kg, entropy of 1.7334 KJ/Kg $^{\circ}\text{K}$ and a volume of 0.09959 m 3 /Kg.

At state 2, the fluid is at a temperature of 25°C as it comes out the compressor as a superheated gas; with a pressure of 0.665605 mpa, enthalpy of 412.33KJ/Kg, entropy of 1.7334 KJ/Kg $^{\circ}\text{K}$ and a volume of 0.03093 m 3 /Kg.

At state 3, the fluid is at a temperature of 15°C as it comes out the condenser as a liquid; with a pressure of 0.665605 mpa, enthalpy of 220.48 KJ/Kg, entropy of 1.07245 KJ/Kg $^{\circ}\text{K}$ and a volume of 0.042115 m 3 /Kg.

At state 4, the fluid is at a temperature of -20°C as it comes out the condenser as a liquid; with a pressure of 0.13273 mpa, enthalpy of 220.48 KJ/Kg, entropy of 0.9002 KJ/Kg $^{\circ}\text{K}$ and a volume of 0.14739 m 3 /Kg.

CONCLUSION

R-134a also known as 1,1,1,2-Tetrafluoroethane is a hydrofluorocarbon that is mainly used in automobiles. Its versatility can be seen throughout the different thermodynamic states. We were tasked with finding the Pressure (P), Enthalpy (H), Entropy (S), and Volume (V) for each state of the refrigeration cycle. We were able to design our refrigeration cycle using the vapor compression diagram and make it work efficiently by applying the first and second Law of Thermodynamics and setting some assumptions. Overall, our refrigerant operated well.

References

Uddin, Kutub. "(PDF) Environmental Assessment and Characteristics of next Generation Refrigerants." ResearchGate, June 2018, www.researchgate.net/publication/326272160_Environmental_Assessment_and_Characteristics_of_Next_Generation_Refrigerants. Accessed 5 Mar. 2022

Abu-Mulaweh, Hosni I., and Abdulaziz A Al-Arfaj. Engineering Design Experience of an Undergraduate Thermodynamics Course. *World Transactions on Engineering and Technology Education*, 1 Nov. 2018.

Smith, J M, et al. *Introduction to Chemical Engineering Thermodynamics*. C, 2018.

AVERAGE

REFRIGERATION CYCLE DESIGN LETTER REPORT

Date: March 4, 2022
To: Professor McIntyre
From: Hillary Ndongo, Breanna, Micheal
Re: Project #1 Design of a Refrigeration cycle

INTRODUCTION

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PROBLEM STATEMENT

A refrigeration system is to be designed to maintain the temperature in the range T_{LOWmin} to T_{LOWmax} , while the outside temperature varies from $T_{HIGHmin}$ to $T_{HIGHmax}$, as given in the team assignment matrix below. The total thermal load on the storage unit is given as 36 kW. Obtain an initial design for the vapor compression refrigeration system shown in Figure 1. Choose a safe and suitable refrigerant. For safe operation and other factors, such as additional energy transfer, design the system using a safety factor of 1.25. The compressor efficiency could range from 60 to 80 percent.

In the course of your design you will need to specify or/and determine the temperatures and pressures at the different states and show the cycle with the vapor dome on a temperature entropy (T-s) diagram or pressure enthalpy (p-H) diagram, or both. Also, you must determine the coefficient of performance value and the mass flow rate of the working fluid.

OBJECTIVE

There were 4 majors focal points for this project:

- Design of the refrigeration system to maintain the following temperature ranges. $T_{Low (min)} = -20^{\circ}\text{C}$, $T_{Low(max)} = -10^{\circ}\text{C}$, $T_{High(min)} = 15^{\circ}\text{C}$ and $T_{High(max)} = 25^{\circ}\text{C}$ and talk about its components and its process.
- Choose a refrigerant with a safety factor of 1.25 and a compressor efficiency that ranges from 60-80% and show the formulas that will be used for our calculations.
- Determine the temperatures and pressures at the different states and show the cycle vapor dome on an T-S diagram or a P-H diagram.

- Determine the coefficient of Performance (cop) value and the mass flow rate of the working fluid.

DESIGN METHODOLOGY

Refrigeration process

A refrigeration cycle has 4 major components:

- Compressor: Its purpose is to circulate the refrigerant in the system. The refrigerant is compressed from a cool gaseous state to a hot high-pressure vapor. Then, the refrigerant moves to the condenser.
- Condenser: Its purpose is to change the hot gas into a liquid. The condenser does so by allowing the high pressure and decrease in temperature to condense the vapor which ejects heat.
- Thermal Expansion Valve: its main purpose is to provide an environment that allows for the refrigerant to decrease in pressure.
- Evaporator: The purpose of the refrigerant is to remove heat which allows for the refrigerant to cool down. Inside the evaporator, the liquid refrigerant is expanded and evaporated.

Assumptions

For the purpose of this project, assumptions need to be made in order to facilitate the calculations:

- The four components operate under steady-state, steady-flow process.
- Both the compressor and the expansion device are considered adiabatic
- Enthalpy $H_3 = H_4$
- Pressure $P_3 = \text{Pressure } P_2$
- Efficiency used = 70%

Procedure and Formulas

For the effectiveness of our design, we utilized a vapor compression refrigeration cycle. Also, we applied the first and second Laws of Thermodynamics while taking in consideration the assumptions mentioned above. See below in table 1, the formulas used:

Table 1

Compressor: Work done in the compressor	$W_{in} = \dot{m}(H_2 - H_1)$
Condenser: Heat released out of the system by the condenser	$Q_{out} = \dot{m}(H_3 - H_2)$

Throttle (Expansion Valve): $H_3 = H_4$	$dS = 0$, $W_{net} = 0$ and $Q_{net} = 0$
Evaporator : Heat entering the evaporator	$Q_{in} = \dot{m}(H_1 - H_4)$
Coefficient of Performance(COP)	$COP = \frac{Q_{in}}{W_{in}}$
Isentropic Entropy	$\eta_c = \frac{W_{ideal}}{W_{actual}} \times 100\%$
Linear Interpolation	$y = y_1 + (x - x_1)((y_2 - y_1)/(x_2 - x_1))$

W_{in} = Power entering the compressor

$\dot{m}$ = Mass flow rate of the refrigerant

Q_{in} = Heat absorbed by the evaporator

Q_{out} = Heat ejected by the condenser

H = Enthalpy

After stating the formulas utilized for our Project, we are going to select our refrigerant.

Refrigerant selection

After considering many refrigerants, we chose R-134A also known as 1,1,1,2-Tetrafluoroethane because it's safe for the environment, easily accessible, it's not highly flammable, safe for humans and convenient to operate at our temperatures.

For the purpose of our project, we will operate within the following given temperatures: T-Low (min) = -20°C, T-Low(max) = -10°C, T-High(min) = 15°C and T-High(max) = 25°C. We also assume an isentropic efficiency of 70% and our refrigerant has a safety factor of 1.25.

The third objective is to show the refrigeration schematic diagram with values for P (Pressure), T (Temperature), H (Enthalpy), S (Entropy) and V (Volumetric Density) at each stage. We will be using the Properties of Saturated table for R-134A and the P-H diagram.

See below Figure 1 representing a schematic diagram of the refrigeration cycle. It shows the major components, the different states (Vapor and/or Liquid), the direction of the refrigerant and Pressure and temperature at different stages. It is also important to underline that we used Linear Interpolation to calculate these values.

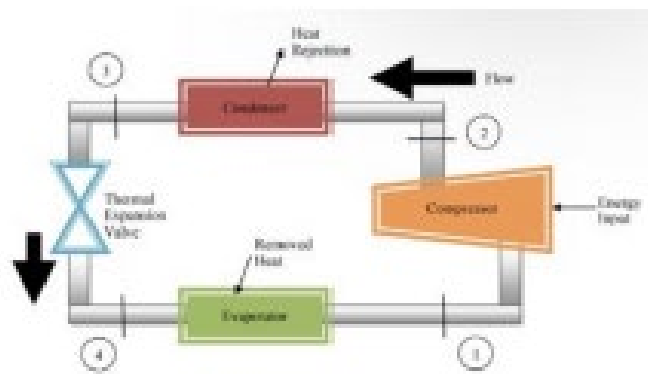


Figure 1: Vapor compression refrigeration cycle

Figure 1: Diagram of Vapor Compression Refrigeration Cycle

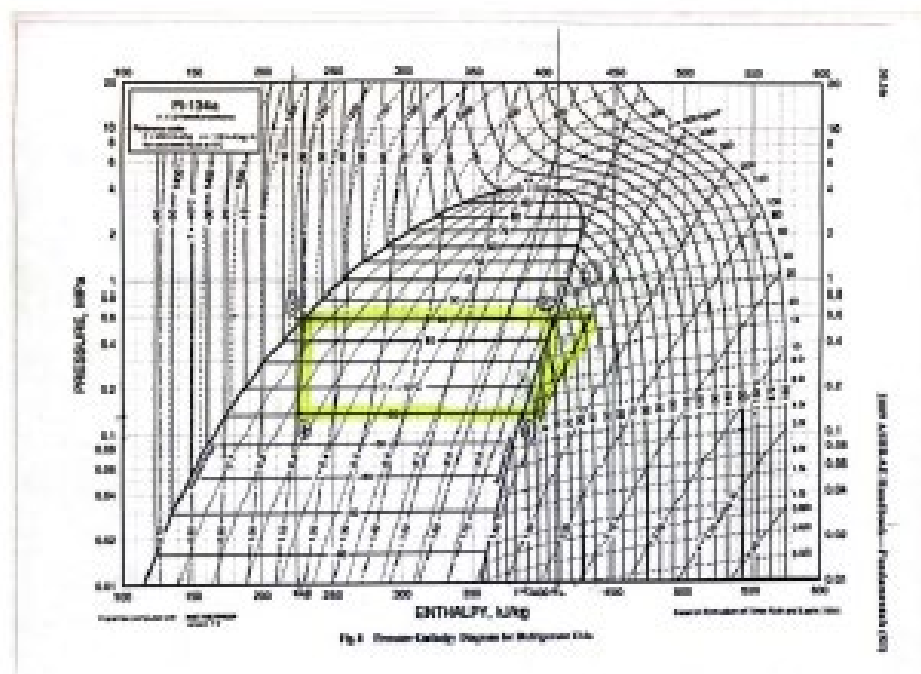


Figure 2: Pressure Enthalpy Diagram For R-134A

RESULTS

As previously mentioned above the values for T , P , H , V and S were obtained from the P-H Diagram and the Properties of Saturated table for R-134A from PVAMU Canvas course Modules. See below a summary of these values at different stages.

	TEMPERATURE °C	PRESSURE (Kpa)	ENTHALPY (KJ/Kg)	ENTROPY (KJ/Kg.K)	x
STATE 1	-25	0.05843	520.99	2.3048	1
STATE 2	25	0.03507	587.90	2.3048	N/A
STATE 3	15	0.25909	234.945	1.12385	N/A
STATE 4	-15	0.089050	166.29	0.8735	0

Q (in)	26
Q (out)	34.46
W _{comp}	8.46
M (kg/s)	0.1895
COP	3.07

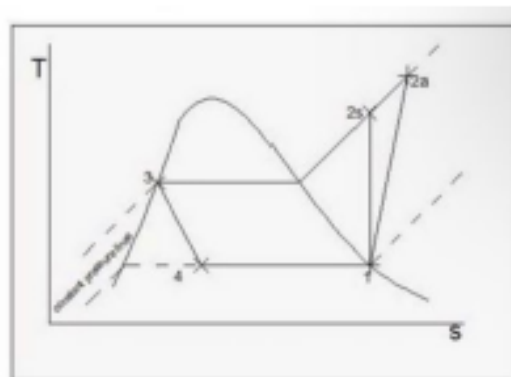


Figure 2: Vapour compression cycle on T-s phase diagram.

DISCUSSION

Figure 1 shows the refrigeration cycle and the states with the corresponding temperatures and pressure.

Figure 2 shows a pressure-enthalpy diagram for R-134a. Based on the diagram, the refrigerant is a saturated vapor at state 1, a superheated gas at state 2, a liquid at state 3, and a liquid-gas mixture at state 4.

Table 1 shows the different components in a refrigeration cycle and their respective equations.

At state 1, the fluid is at a temperature of -25°C as it comes out the evaporator as a saturated vapor; with a pressure of 0.05843 mpa, enthalpy of 520.99 KJ/Kg, entropy of 2.3048 KJ/Kg $^{\circ}\text{K}$ and a volume of 0.59062 m^3/Kg .

At state 2, the fluid is at a temperature of 25°C as it comes out the compressor as a superheated gas; with a pressure of 0.3507 mpa, enthalpy of 587.90KJ/Kg, entropy of 2.3048KJ/Kg $^{\circ}\text{K}$ and a volume of 0.109579 m^3/Kg . At state 3, the fluid is at a temperature of 15°C as it comes out the condenser as a liquid; with a pressure of 0.25909 mpa, enthalpy of 234.945 KJ/Kg, entropy of 1.12385 KJ/Kg $^{\circ}\text{K}$ and a volume of 0.14648 m^3/Kg .

At state 4, the fluid is at a temperature of -15°C as it comes out the condenser as a liquid; with a pressure of 0.089050 mpa, enthalpy of 166.29 KJ/Kg, entropy of 0.8735 KJ/Kg $^{\circ}\text{K}$ and a volume of 0.39904 m^3/Kg .

CONCLUSION

R-600a Isobutane is a hydrofluorocarbon that is mainly used in automobiles. Its versatility can be seen throughout the different thermodynamic states. We were tasked with finding the Pressure (P), Enthalpy (H), Entropy (S), and Volume (V) for each state of the refrigeration cycle. We were able to design our refrigeration cycle using the vapor compression diagram and make it work efficiently by applying the first and second Law of Thermodynamics and setting some assumptions. Overall, our refrigerant operated well.

References

Uddin, Kutub. "(PDF) Environmental Assessment and Characteristics of next Generation Refrigerants." *ResearchGate*, June 2018, www.researchgate.net/publication/326272160_Environmental_Assessment_and_Characteristics_of_Next_Generation_Refrigerants. Accessed 5 Mar. 2022

Abu-Mulaweh, Hosni I., and Abdulaziz A Al-Arfaj. *Engineering Design Experience of an Undergraduate Thermodynamics Course*. World Transactions on Engineering and Technology Education, 1 Nov. 2018.

Smith, J M, et al. *Introduction to Chemical Engineering Thermodynamics*. C, 2018.

BELOW AVERAGE

Date: March 04, 2022
To: Professor E. Carl McIntyre
From: Wilfried Zagre

THE REFRIGERATION CYCLE

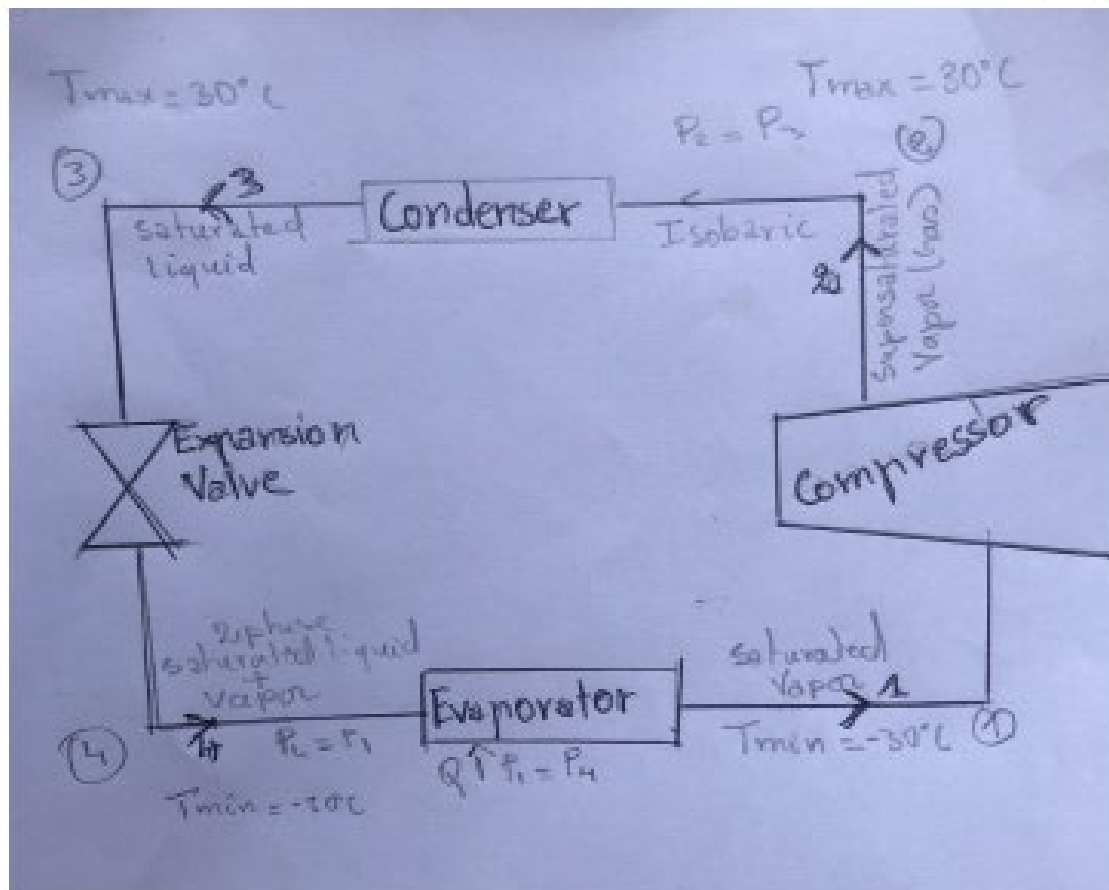
ABSTRACT

The refrigeration cycle is a thermodynamic process where a fluid absorbs thermal energy from the surrounding at a low temperature but ejects the same thermal energy to the surrounding at a higher temperature. This project will clarify the refrigeration cycle design while meeting the desired needs. For this project to be successful, some thermodynamic laws would be used such as the first and second laws of thermodynamics, isentropic compressor efficiency and coefficient of performance, etc. We have been exposed with few requirements to accomplish the project the following states:

- Design a refrigeration system to maintain given temperature ranges from -25°C to 25°C
- Choose a safe and suitable refrigerant given a contingency factor of 1.3
- Determine temperatures and pressures at different states
- Show the cycle on a pressure-enthalpy/temperature-entropy (P - H or T - S) diagram
- Determine the coefficient of performance (COP) value
- Determine the mass flow rate of the working fluid.

INTRODUCTION

There are generally four components in a refrigeration cycle, and they are an evaporator, a compressor, a condenser, and a thermal expansion valve. For cooling to occur, the refrigerant passes through all 4 components. As engineers we know that heat transfer occurs from areas of high temperatures to areas of low temperatures, this is also true and applies for the refrigeration cycle. To explain what happens in each component of the refrigeration system, we came up with a handmade sketch below with detail temperatures and few states established that we would implement better in the recorded video:



For our project, we choose to operate with (R-407C). This refrigerant is a zeotropic blend made from a mixture of hydrofluorocarbons to the likes of difluoromethane, pentafluoro-ethane, and 1,1,1,2-tetrafluoromethane.

The Evaporator

We picked this component first because it is the first stage that the blend goes through its first transformation. As the name implies, an evaporator is a device used in the conversion of a substance from its liquid phase to its corresponding gaseous phase. So, air cannot leak into the refrigeration system, the vapor pressure of the refrigerant at the evaporator temperature should be greater than atmospheric pressure. The Evaporator removes heat from the interior of the refrigerator compartment by exchanging heat between the air inside the refrigerator and the refrigerant passing through the tubes of the evaporator. In the refrigeration cycle, a two-phase fluid containing liquid, and vapor makes its way into the evaporator and at the injection of heat into the

evaporator, a saturated vapor is released to the condenser. It is important to know that the process in the evaporator is an isobaric process because it occurs at constant pressure ($\Delta P=0$).

The Compressor

The cycle requires input of power to increase the pressure of a gas. The refrigerant enters at low pressure and low temperature in a gaseous form. It cannot operate on liquids; the working fluid must leave the evaporator and enter the compressor at least as saturated vapor. This is an adiabatic process and is Isentropic, therefore the change in entropy is zero ($\Delta S=0$). Another goal we considered in this project was the isentropic efficiency(η) of the compressor which we would discuss below. An important concept in the operation of a compressor is the conversion of saturated vapor to superheated gas.

The Condenser

This device is also a heat exchange device and transfers heat between two different fluids. The condenser is used to remove heat gained from the refrigerant through the evaporator and the compressor. The transfer of heat to the ambient air must be at a lower temperature than that of the refrigerant exiting the condenser. The condenser occurs in an isobaric condition and in this condition, it converts superheated gas to saturated liquid.

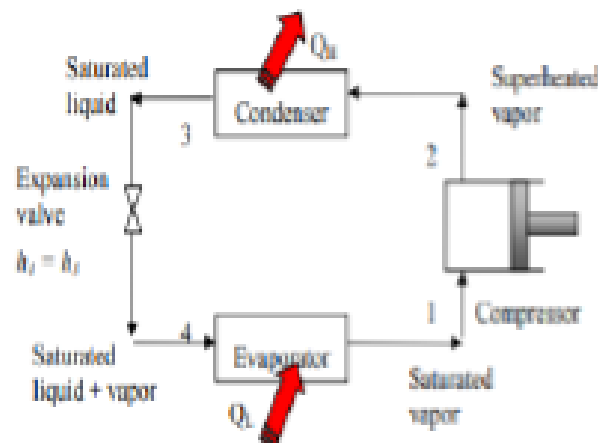
The Thermal Expansion Valve

Controls the amount of refrigerant flow into the evaporator and controls the superheating at the outlet of the evaporator. Two phases occur here: saturated liquid and saturated vapor. There's no change in enthalpy and pressure is constant.

Now with our knowledge of the refrigeration cycle, it's time to start the project.

PROBLEM STATEMENT:

A refrigeration system is to be designed to maintain the temperature in the range -25°C to -15°C , while the outside temperature varies from 15°C to 25°C . The total thermal load on the storage unit is given as 33kW. Obtain an initial design for the vapor compression refrigeration system shown in Figure 1. Choose a safe and suitable refrigerant. For safe operation and other factors, such as additional energy transfer, design the system using a safety factor of 1.3. The compressor efficiency could range from 60 to 80 percent.



ASSUMPTIONS

Here are our assumptions:

- This is an open system because there's a total exchange and insignificant loss of energy
- It operates under steady-state and steady-flow processes
- Kinetic and Potential energies across each device is negligible
- Compressor and expansion devices are adiabatic,
- Evaporator and condenser are considered constant pressure devices i.e., isobaric
- The isentropic efficiency of the compressor was selected to be 60%.

For this project, we choose to operate with (R-407C). This refrigerant is a zeotropic blend made from a mixture of hydrofluorocarbons to the likes of difluoromethane, pentafluoro-ethane, and 1,1,1,2-tetrafluoromethane. Some of the factors that made R407C a viable option is that R-407C has zero ozone depletion potential making it less harmful to our environment, it is relatively cheap considering its market value is at \$4-\$7 per pound and it works in medium temperature refrigeration systems like most air conditioners. The freezing point of Difluoromethane is -160°C which means it's less than our T-Low (min), -25°C . It has a critical temperature (86.0°C) that is higher than the atmospheric temperature of the earth and has a boiling point of -43.6°C .

P-H DIAGRAM

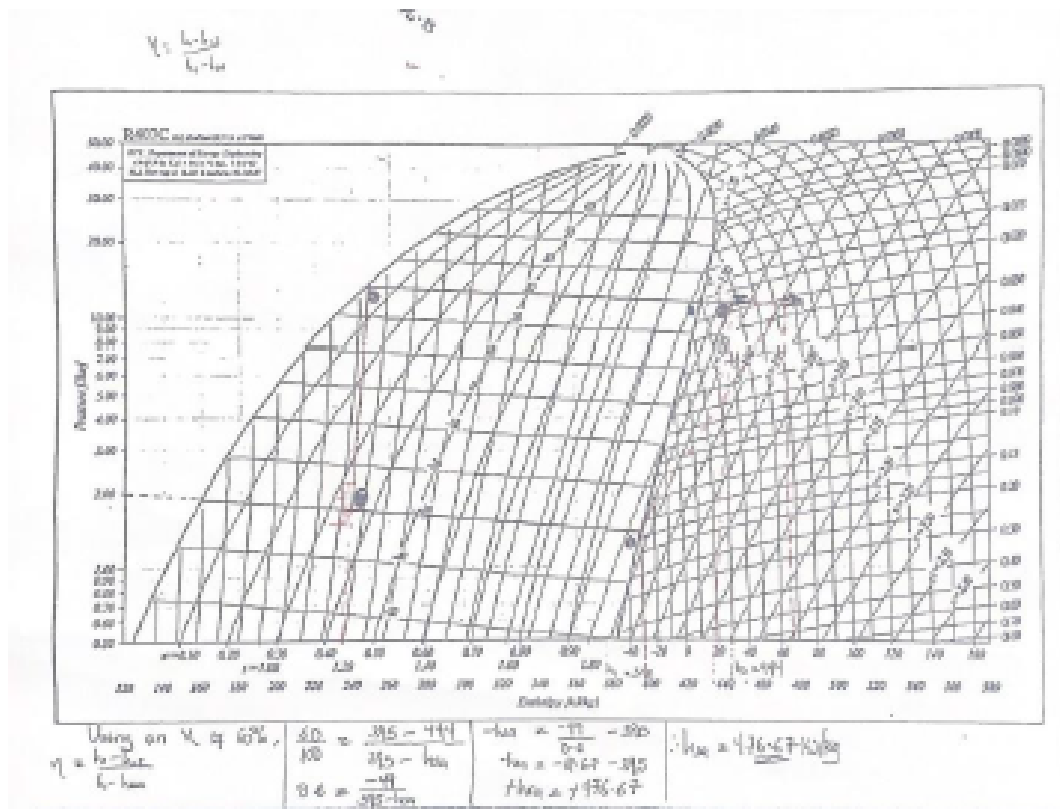


Table 1: Thermodynamic values:

State	T (°C)	P (kPa)	P(bar)	H (kJ/kg)	S (kJ/kg.K)
1	-30	1.48	2	395	1.82
2s	30	20.12	15	444	1.82
2a	30	20.12	15	476.67	1.91
3	30	20.12	15	232	0
4	-30	1.48	2	232	1.18

Using the P-H diagram we were able to input the values in Table 1. Using the table above, we calculated the value for h_{2a} as shown below:

The Refrigeration Cycle

Group II 6

$$h_{2a} = \frac{(h_{2a} - h_1)}{.60} + h_1$$

$$h_{2a} = \frac{(444 - 398)}{.60} + 398 = 476.67 \text{ kJ/kg}$$

Table 2: Design values.

Q_{in}	42.9
Q_{out}	63.12
W_s	20.29
$\dot{m}(\text{kg/s})$	.26
COP	2.02

To fill out Table 2, we used the following formulas:

From the problem statement we were given that our thermal load is 33kW and a factor of safety of 1.3. If we multiply 33 by 1.3, we get a cooling load of 42.9kW.

We know the formula for an open system is:

$$\Delta H + E_k + E_p = Q + W$$

For our refrigeration system the kinetic and potential energies across each device is negligible.

i.e., $E_p = 0$, $E_k = 0$

So, our formula now is:

$$\Delta H = Q + W$$

We now apply this formula over each component.

Evaporator: $\Delta H = Q + W_s$ (there's no work done here because of constant pressure, so $W_s = 0$)

So, we use this formula: $\Delta H = Q_{in}$

$$\dot{m} = \frac{Q_{in}}{(h_1 - h_4)}$$

$$\dot{m} = \frac{42.9}{(398 - 23.2)}$$

$$\dot{m} = .26 \text{ kg/s}$$

Compressor: $\Delta H = Q + W_s$ (this is adiabatic, so $Q = 0$)

So, we use this formula: $\Delta H = W_s$

$$\dot{m} (h_{2a} - h_1) = W_s$$

$$.26 (476.67 - 398) = 21.23 \text{ J}$$

Condenser: $\Delta H = Q + W_s$ (this is an isobaric process, $W_s = 0$)

The Refrigeration Cycle

Group II 7

So, we use this formula: $\Delta H = Q$

$$\dot{m} (h_{2a} - h_2) = Q_{out}$$
$$.26 (476.67 - 232) = 63.61J$$

COP: Coefficient of Performance

$$COP = \frac{Q_{in}}{W}$$
$$COP = \frac{42.9}{21.23} = 2.02$$

I chose to use 60% for our efficiency but having all this data let's prove the isentropic efficiency of the compressor. The formula is:

$$\eta = \frac{h_1 - h_{2s}}{h_1 - h_{2a}}$$
$$= \frac{393 - 444}{393 - 476.67}$$
$$\eta = .60 = 60\%$$

CONCLUSION

This project was given to test our understanding of the concepts and principles of what we've covered so far in Thermodynamics I and Thermodynamics II. I believe this project will allow us to understand the concepts of thermodynamics II while covering the class. With all the resources offered by Dr McIntyre, we were able to follow the process of the refrigerant chosen and their efficiency in the project. The paper by Al-Arfaj and Abu-Mulaweh and Chemical Engineering Thermodynamics, 8th edition book offered was a big help toward accomplishing this project.

This concludes the assignment.

Respectfully submitted,

Wilfried Zagre
Student of the Chemical Engineering Department
Spring 2022

References

The Refrigeration Cycle

Group II 8

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[210907 c y b refrigerant thermophysical properties SI F09 Ch30.pdf](#)

[210405 sample reporting guidance.docx](#)

CHEMICAL ENGINEERING THERMODYNAMICS II

SPRING 2022

Title of Assignment: UPLOAD LETTER REPORT FOR PROJECT 2
Using ASPEN Simulation for Txy, Pxy Diagram Generation and
Activity Coefficient Model Selection

TOPICS COVERED IN PROJECT 2

Project 2 covered the following topics:

1. Literature search to find published VLE data for binary systems
2. Ideal solution behavior and departure from Raoult's Law
3. Activity coefficient models accounting for non-ideal solution behavior
4. Generation of phase diagrams (Txy and Pxy) using ASPEN.
5. Comparison of model simulations of phase behavior with real data obtained from the published literature
6. Selection of the best model based on visual observation of overlaid data and theory plots
7. Experience working in teams
8. Written communication

Using ASPEN Simulation for T-x-y, P-x-y Diagram Generation and Activity Coefficient Model Selections

This activity builds on what we have been learning in class about activity coefficients and how they can be modeled. It introduces you to chemical process simulation through use of built in property packages, which need to be specified in order to do a simulation with your particular set of components. A learning outcome will be that you will be able to calculate VLE data for a binary system and used it to model separation (and other operations) of a process stream using a chemical process simulation package from AspenTech, Inc. To help you become experienced users of ASPEN, you will use it to create the phase diagrams that you have been working much of this semester. Also, you will gain some experience with property method selection by comparing ASPEN simulation results with different choices of method.

So, this project occurs in three phases including the following activities: literature search in which you will select a binary system, acquire a table of published VLE data, and gain approval from instructor; use of ASPEN to generate Txy and Pxy diagrams for the system and conditions you had approved; and use of ASPEN to simulate your system using different property methods (such as Ideal Solution, Peng Robinson, etc.) and make comparison of simulation results with published VLE data; and reporting.

Instructional Objectives – At the end of this exercise, students will be able to accomplish the following.

- Use sources published information such as Perry's Handbook and online sources including the Internet search engines such as Google Scholar, and data base indexes such as Compendex.
- Select a binary system with useful VLE data.
- Reinforce knowledge of a simple flash drum separator
- Generate phase diagrams using the ASPEN simulator.
- Select a thermodynamics package to model a binary system.
- Compare simulation results to published data on binary system VLE

Because of the scope of information that must be searched, and the different skills required to complete this project, you are required to work in teams. Your instructor will allow you to form your team assignments. Do so by selecting the same team in Canvas as your team mates do (use the People link, and the Project2 tab, or send a message to your instructor with your teaming preference). When assigned, teaming will appear in Table 1.

An overview of the procedure you will use in making a simulation is outlined below.

Phase 1

- There are multiple sources of the data you will need. It will be best to use your team to "divide and conquer" the territory. You must find a set of data for VLE of a binary system that includes a table of P-x-y or T-x-y data. Each team will have a different binary system, so your selection is not final until approved by the instructor. Ideal binary systems are not allowed.
- Use the attached ASPEN Cookbook for VLE Calculation to practice generating T-x-y and P-x-y diagrams.

Phase 2

- Apply the technique learned in Phase 1 to use ASPEN for generating phase diagrams predicting VLE behavior, for various activity coefficient models.
- Compare the results of the ASPEN model predictions for your system to the actual data you obtained from your literature study in Phase 1. Find the model that best fits the data.

Phase 3

- Submit results via *eCourses*. All submissions will be via *eCourses*.
 - No cover page.
 - Deliverable is a letter report written in MSWord, with letter style formatting of address block; message body explaining assignment and attachments, along with a quick description of results; and signature block including all teammates who participated.

- Files attached as an appendix: (1) report containing table experimental data; figures based on ASPEN screenshots (with appropriate captions) or plotted data from ASPEN report files; plots showing comparisons of simulation results to actual data; findings, conclusions, and references; supporting literature, ASPEN simulation, and ASPEN report files.

NOTE: You will need a way to access ASPEN. **It is available for you to run from the Wilson 202 computer lab, which is the default access mode for this face-to-face course.** If you would like to access it remotely, you will need to use VDI or VPN. Contact technical support if you need remote access.

Aspen Cookbook for VLE Calculations

1. Select blank simulation, OK.
2. Select local PC, OK.
3. Select the units: Click on Data, Setup, Input data: Output results:, then close window.
4. Click on Separators, click on Flash2, place in the middle of the canvas.
5. Click on Material STREAMS, connect the required streams on the Flash drum (red), Feed, Vapor, Liquid.
6. Rename the streams, select (left click) then right click, rename.
7. Data, Components, Specifications: type in names, e.g., Methanol, then propane, etc.
8. Data, Properties, Specifications, Base Method, select PENG-ROB or some other method. Note that a brief description appears in the bottom pane when your mouse is over a given method.
9. Data, Setup, Report Options, Stream tab, select all items to be included in the report.
10. Select, right click on Feed stream, Input. Specify T, P, composition, flow rate and anything else you need.
11. Select, right click on Flash, Input. Specify the Flash Temperature and vapor fraction (change Pressure to Vapor fraction). Be sure that your temperature is below the critical point of the mixture or you will not get a flash calculation.
12. Data, Properties, Prop-sets, New → name it, find PHIMX, etc. and add as many properties to that prop-set that you need. Then click on the Qualifiers tab, select liquid in one column and vapor in the second column. You do not need to select a component.
13. Add the property set to the report: Data, Setup, Report options, Stream, Property Sets, find the name and add it.
14. Do the calculation. You need to do this even though you are not interested in the results. Run, Run, or N →.
15. You can now view the results of the calculation. Click on Check results in the Control Panel (blue folder with blue check mark).
16. If you want to generate Pxy or Txy diagrams: Tools, Analysis, Property, Binary, generate Pxy or Txy or Gibbs.
17. Select Analysis type: Pxy (or Txy)
18. Select temperature (or pressure).
19. Change the number of points or composition range, etc. @ if desired.
20. Click on Go.
21. To select a different property method (e.g., NRTL, etc.) go to step 8 and then re-run the flash calculation.
22. View the results.

**CHEMICAL ENGINEERING THERMODYNAMICS II
SPRING 2022**

**SAMPLE WRITTEN REPORTS SUBMITTED AND
AND GRADING SCHEME FOR PROJECT 2**

ABOVE AVERAGE

USING DWSIM SIMULATION FOR T-x-y, P-x-y DIAGRAM GENERATION AND ACTIVITY COEFFICIENT MODELS SELECTION FOR BINARY MIXTURE: TOLUENE AND 1-BUTANOL

Date: May 4th, 2022

To: Professor McIntyre

From: Laury Mengue

Re: Project #2 Pxy- Txy diagrams for Toluene and 1-Butanol

INTRODUCTION

In materials chemistry, a binary phase or binary compound is a chemical compound containing two different elements. For the purpose of our project we will use the following binary system: **Toluene and 1-Butanol**. Simulating the T-xy and P-xy diagrams of this mixture allow us to know the nature and composition of each phase of the mixture that is present.

PROBLEM STATEMENT

This activity builds on what we have been learning in class about activity coefficients and how they can be modeled. It introduces you to chemical process simulation through use of built in property packages, which need to be specified in order to do a simulation with your particular set of components. A learning outcome will be that you will be able to calculate VLE data for a binary system and use it to model separation (and other operations) of a process stream using a chemical process simulation package from DWSIM To help you become experienced users of DWSIM, you will use it to create the phase diagrams that you have been working much of this semester. Also, you will gain some experience with property method selection by comparing DWSIM simulation results with different choices of method.

So, this project occurs in three phases including the following activities: literature search in which you will select a binary system, acquire a table of published VLE data, and gain approval from instructor; use of DWSIM to generate Txy and Pxy diagrams for the system and conditions you had approved; and use of DWSIM to simulate your system using different property methods (such as Ideal Solution, Peng Robinson, etc.) and make comparison of simulation results with published VLE data; and reporting.

OBJECTIVES

The objectives for this project are as followed:

- Use sources published information such as Perry's Handbook and online sources including the Internet search engines such as Google Scholar, and database indexes such as Compendex.
- Select a binary system with useful VLE data.
- Reinforce knowledge of a simple flash drum separator
- Generate phase diagrams using the DWSIM simulator.
- Select a thermodynamics package to model a binary system.

- Compare simulation results to published data on binary system VLE

GIVEN CONDITIONS

For the purpose of this report, the following conditions are set:

- Temperature $T = 363.15 \text{ K} = 90^\circ \text{C}$
- Pressure $P = 760 \text{ mmHg} = 101.325 \text{ KPa}$
- Models used are: Wilson Model, UNIFAC Model and Peng-Robinson Model
- DWSIM simulation software is used in lieu of ASPEN

METHODS USED

For the purpose of our project, the following 3 methods will be used:

- Wilson : The Wilson equation is used to predict the activity coefficients γ_1 and γ_2 over the range of liquid compositions
- UNIFAC: The UNIFAC method is a semi-empirical system for the prediction of non-electrolyte activity in non-ideal mixtures
- Peng Robinson: The Peng-Robinson equation of state can be used to determine the enthalpy and entropy of a fluid or fluid mixture provided that the specific heat of the pure fluid(s) in the ideal gas state is known as a function of temperature.

RESEARCH PAPER GRAPHS AND DATA

The research paper used as a comparison base for this project is initially analysis to the ternary vapor-liquid equilibrium data of the system methylcyclohexane-toluene-n-butanol. However, the binary vapor- liquid equilibrium data of the system Toluene and -1-butanol have been determined. See below the VLE data (Also see attached appendix A):

Table 101
Toluene-Toluene (1) and Butanol (2)
Vapor-liquid equilibrium at 101 mm Hg

Run no.	Temp., °C Temp., °F	Temp., °C Temp., °F	x_1	y_1	γ_1	γ_2	γ_1	γ_2	γ_1	γ_2
Toluene-Toluene (1) and Butanol (2)	100.0	212.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	110.0	230.0	0.05	0.05	1.05	1.05	1.05	1.05	1.05	1.05
	120.0	248.0	0.1	0.1	1.1	1.1	1.1	1.1	1.1	1.1
	130.0	266.0	0.15	0.15	1.15	1.15	1.15	1.15	1.15	1.15
	140.0	284.0	0.2	0.2	1.2	1.2	1.2	1.2	1.2	1.2
	150.0	302.0	0.25	0.25	1.25	1.25	1.25	1.25	1.25	1.25
	160.0	320.0	0.3	0.3	1.3	1.3	1.3	1.3	1.3	1.3
	170.0	338.0	0.35	0.35	1.35	1.35	1.35	1.35	1.35	1.35
	180.0	356.0	0.4	0.4	1.4	1.4	1.4	1.4	1.4	1.4
	190.0	374.0	0.45	0.45	1.45	1.45	1.45	1.45	1.45	1.45
Toluene-Toluene (1) and Butanol (2)	200.0	392.0	0.5	0.5	1.5	1.5	1.5	1.5	1.5	1.5
	210.0	410.0	0.55	0.55	1.55	1.55	1.55	1.55	1.55	1.55
	220.0	428.0	0.6	0.6	1.6	1.6	1.6	1.6	1.6	1.6
	230.0	446.0	0.65	0.65	1.65	1.65	1.65	1.65	1.65	1.65
	240.0	464.0	0.7	0.7	1.7	1.7	1.7	1.7	1.7	1.7
	250.0	482.0	0.75	0.75	1.75	1.75	1.75	1.75	1.75	1.75
	260.0	500.0	0.8	0.8	1.8	1.8	1.8	1.8	1.8	1.8
	270.0	518.0	0.85	0.85	1.85	1.85	1.85	1.85	1.85	1.85
	280.0	536.0	0.9	0.9	1.9	1.9	1.9	1.9	1.9	1.9
	290.0	554.0	0.95	0.95	1.95	1.95	1.95	1.95	1.95	1.95
Toluene-Toluene (1) and Butanol (2)	300.0	572.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	310.0	590.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	320.0	608.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	330.0	626.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	340.0	644.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	350.0	662.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	360.0	680.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	370.0	698.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	380.0	716.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	390.0	734.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0

Vapor-liquid equilibrium at 101 mm Hg

Run no.	Total pressure, mm. Hg	Total pressure, mm. Hg	x_1	y_1	γ_1	γ_2	γ_1	γ_2	γ_1	γ_2
Toluene-Toluene (1) and Butanol (2)	100.0	212.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	110.0	230.0	0.05	0.05	1.05	1.05	1.05	1.05	1.05	1.05
	120.0	248.0	0.1	0.1	1.1	1.1	1.1	1.1	1.1	1.1
	130.0	266.0	0.15	0.15	1.15	1.15	1.15	1.15	1.15	1.15
	140.0	284.0	0.2	0.2	1.2	1.2	1.2	1.2	1.2	1.2
	150.0	302.0	0.25	0.25	1.25	1.25	1.25	1.25	1.25	1.25
	160.0	320.0	0.3	0.3	1.3	1.3	1.3	1.3	1.3	1.3
	170.0	338.0	0.35	0.35	1.35	1.35	1.35	1.35	1.35	1.35
	180.0	356.0	0.4	0.4	1.4	1.4	1.4	1.4	1.4	1.4
	190.0	374.0	0.45	0.45	1.45	1.45	1.45	1.45	1.45	1.45
Toluene-Toluene (1) and Butanol (2)	200.0	392.0	0.5	0.5	1.5	1.5	1.5	1.5	1.5	1.5
	210.0	410.0	0.55	0.55	1.55	1.55	1.55	1.55	1.55	1.55
	220.0	428.0	0.6	0.6	1.6	1.6	1.6	1.6	1.6	1.6
	230.0	446.0	0.65	0.65	1.65	1.65	1.65	1.65	1.65	1.65
	240.0	464.0	0.7	0.7	1.7	1.7	1.7	1.7	1.7	1.7
	250.0	482.0	0.75	0.75	1.75	1.75	1.75	1.75	1.75	1.75
	260.0	500.0	0.8	0.8	1.8	1.8	1.8	1.8	1.8	1.8
	270.0	518.0	0.85	0.85	1.85	1.85	1.85	1.85	1.85	1.85
	280.0	536.0	0.9	0.9	1.9	1.9	1.9	1.9	1.9	1.9
	290.0	554.0	0.95	0.95	1.95	1.95	1.95	1.95	1.95	1.95
Toluene-Toluene (1) and Butanol (2)	300.0	572.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	310.0	590.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	320.0	608.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	330.0	626.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	340.0	644.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	350.0	662.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	360.0	680.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	370.0	698.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	380.0	716.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0
	390.0	734.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0

T-xy plot Diagram for Toluene and 1- Butanol

Fig. 1.

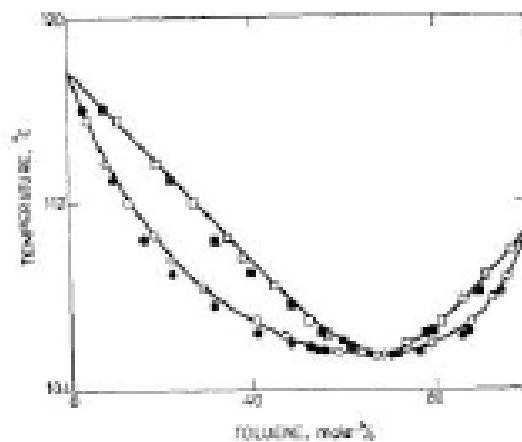


Fig. 1. *T-x-y* diagram for system: Toluene-*n*-Butanol at 760 mm Hg

Liquid Vapour
 ○ — this work □ — this work
 ● — Mann & Shonlit ■ — Mann & Shonlit

From the plot, we can estimate the T_{sat} for Butanol to be roughly 117°C . Also, the T_{sat} for Toluene is roughly 110°C .

Plot of X-Y mole fraction of Toluene at the given conditions given above

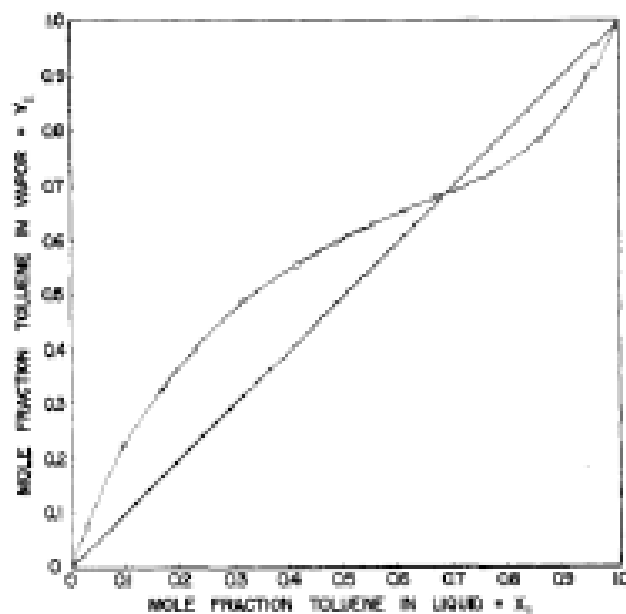


Figure 2. Vapor liquid equilibrium curve for *n*-butanol-toluene system

Plot of Activity Coefficient Diagram

It's important to specify that Margules equation parameters were used to calculate the Activity Coefficients γ_1 and γ_2 .

See below a table of the Parameters A_{12} and A_{21} and a plot of the Activity Coefficient Diagram

TABLE V				
End-values of activity coefficients for both systems at 90°C and 760 mm Hg				
System	End values		Average error, %	
	A_{12}	A_{21}		
Methylcyclohexane- <i>n</i> -butanol	0.44	0.68	1.93	2.16
	0.56	0.10	2.0	2.34
Toluene- <i>n</i> -butanol	0.60	0.45	1.33	1.64
	0.40	0.33	1.16	1.10

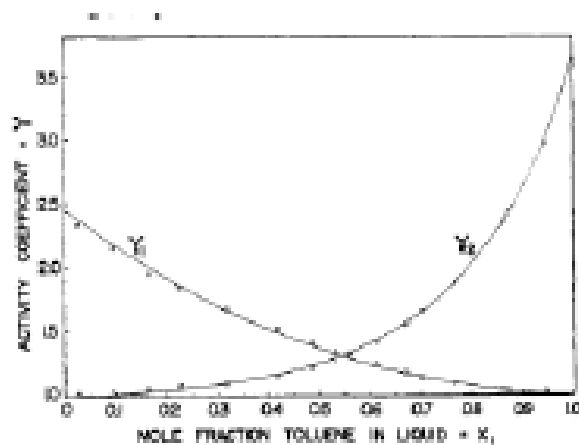
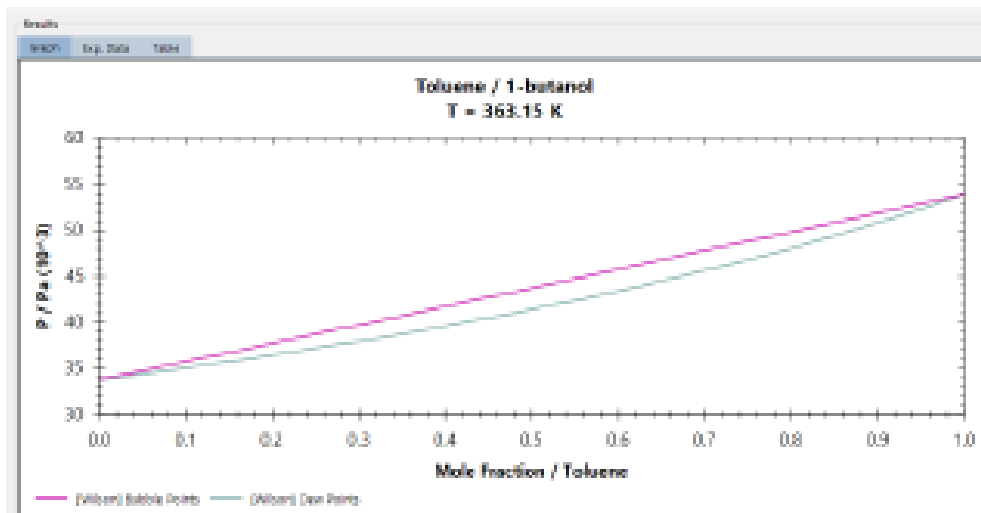


Figure 3. Activity coefficient-composition curve for 1-butanol-toluene system

From the graph, both activity coefficient curves meet roughly at X_1 (Mole fraction of Toluene Liquid) is roughly 0.54. The curve from γ_1 goes from roughly 2.5 to 1 and the curve for γ_2 goes from 1 to roughly 3.7.

SIMULATION GRAPHS AND DATA USING DWSIM

Wilson P-xy

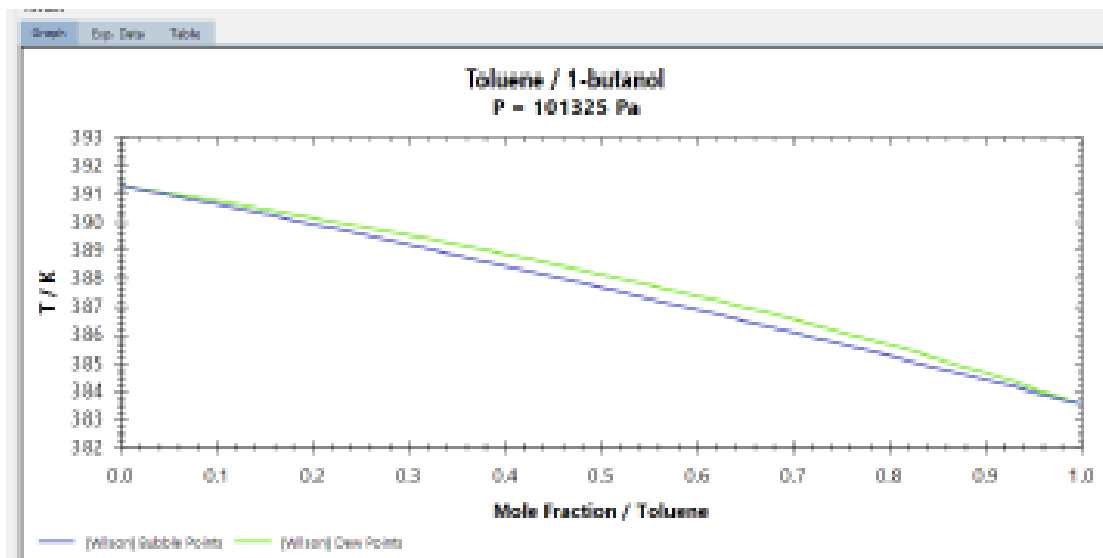


Using the Wilson Model, the P-xy graph shows that:

Psat(1-Butanol) = 34 KPa

Psat (Toluene) = 54 KPa

Wilson T-xy

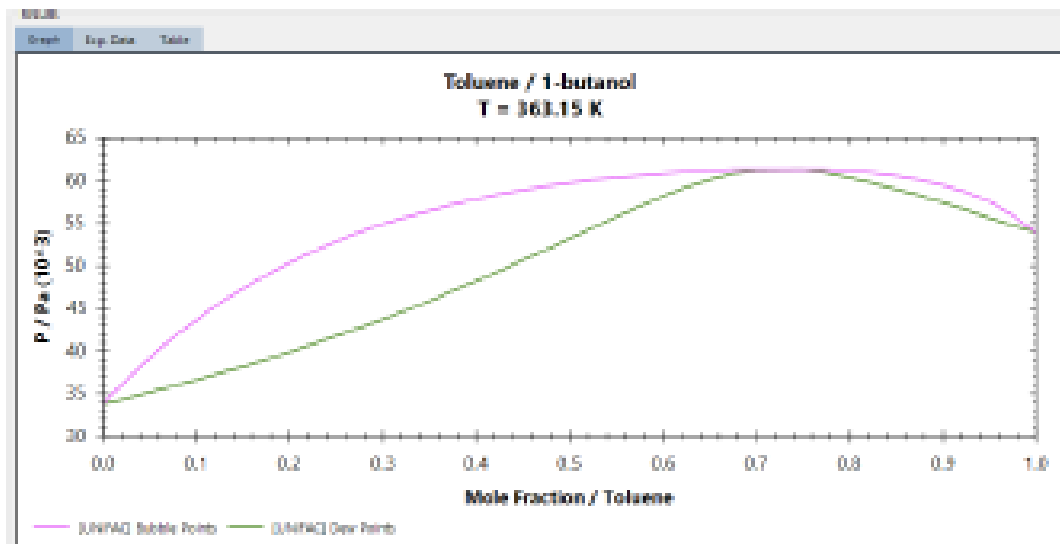


Using the Wilson Model, the T-xy graph shows that:

Tsat(1-Butanol) = 391.2 K

Tsat (Toluene) = 383.6 K.

UNIFAC P-xy

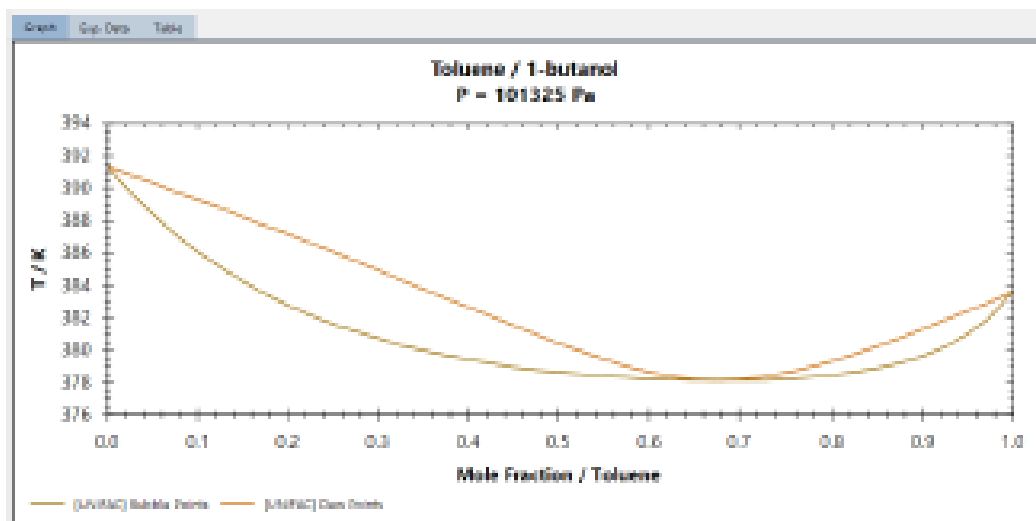


Using the UNIFAC Model, although the P-xy graph looks different from the one obtained by the Wilson model, the results are still the same.

$P_{\text{sat}}(\text{1-Butanol}) = 34 \text{ KPa}$

$P_{\text{sat}}(\text{Toluene}) = 54 \text{ KPa}$

UNIFAC- T-xy

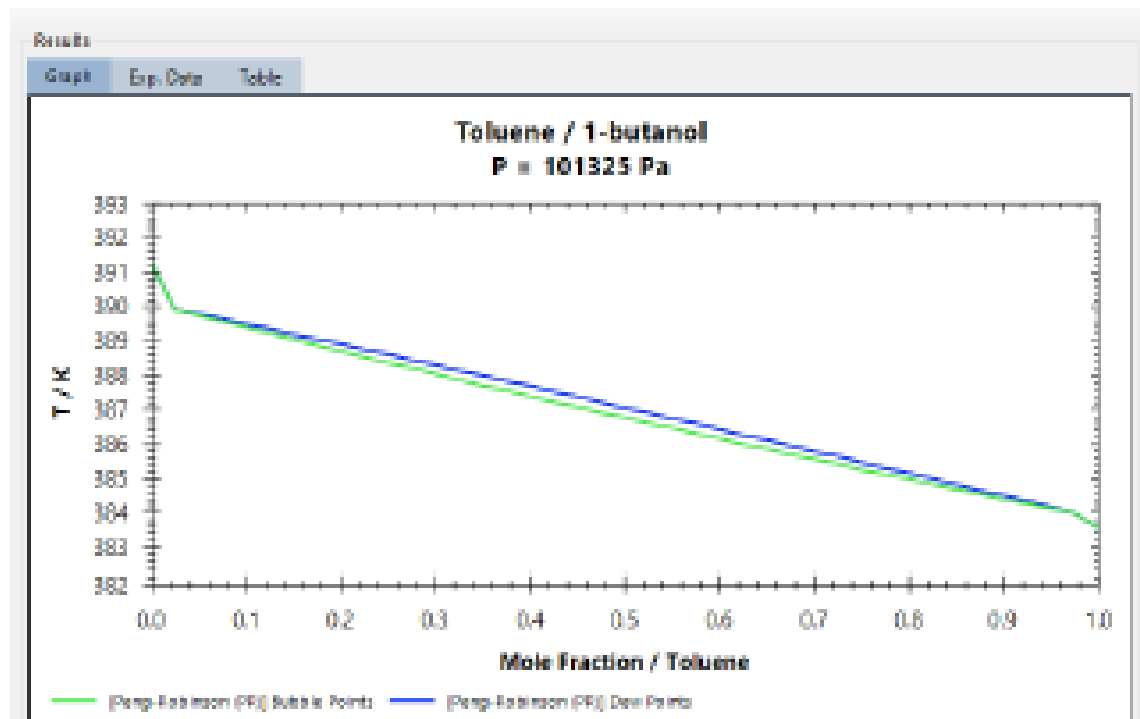


Using the UNIFAC Model, the T-xy graph shows that:

$T_{\text{sat}}(\text{1-Butanol}) = 391.2 \text{ K}$

$T_{\text{sat}}(\text{Toluene}) = 383.6 \text{ K}$

Peng- Robinson Model T-xy

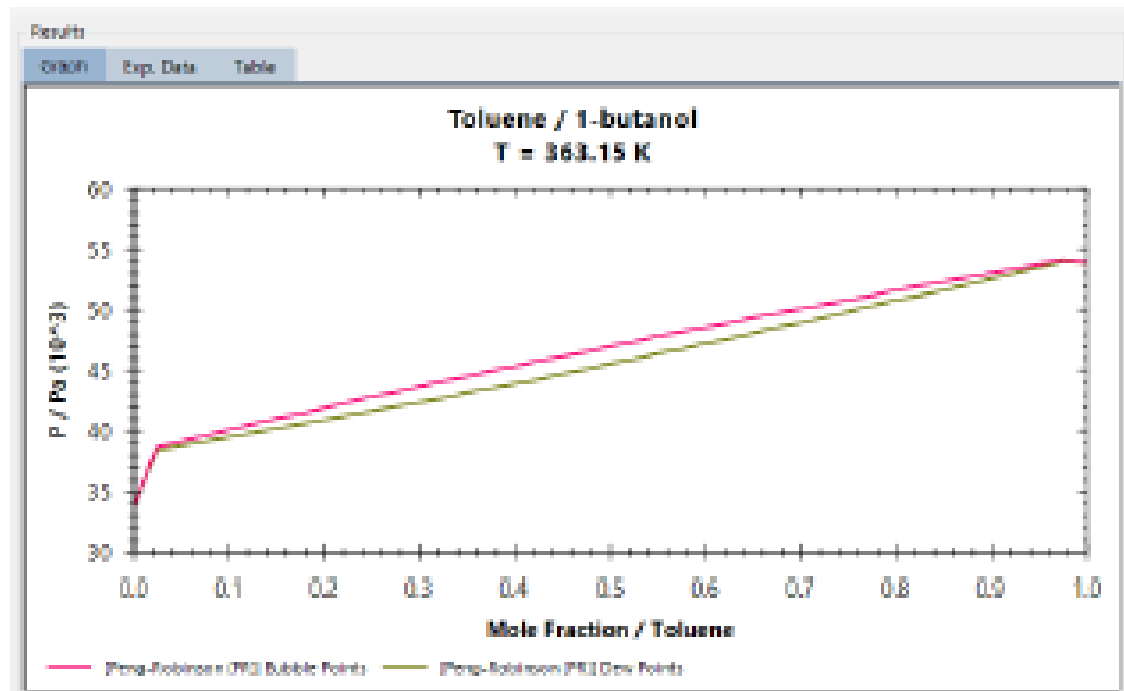


Using the PR Model, the T-xy graph shows that:

Tsat(1-Butanol) = 391.2 K

Tsat (Toluene) = 383.6 K.

Peng- Robinson Model P-xy



Using the PR Model, the P-xy graph shows that:

Tsat(1-Butanol) = 34 KPa

Tsat (Toluene) = 54 KPa

Simulation data obtained in DSWIM

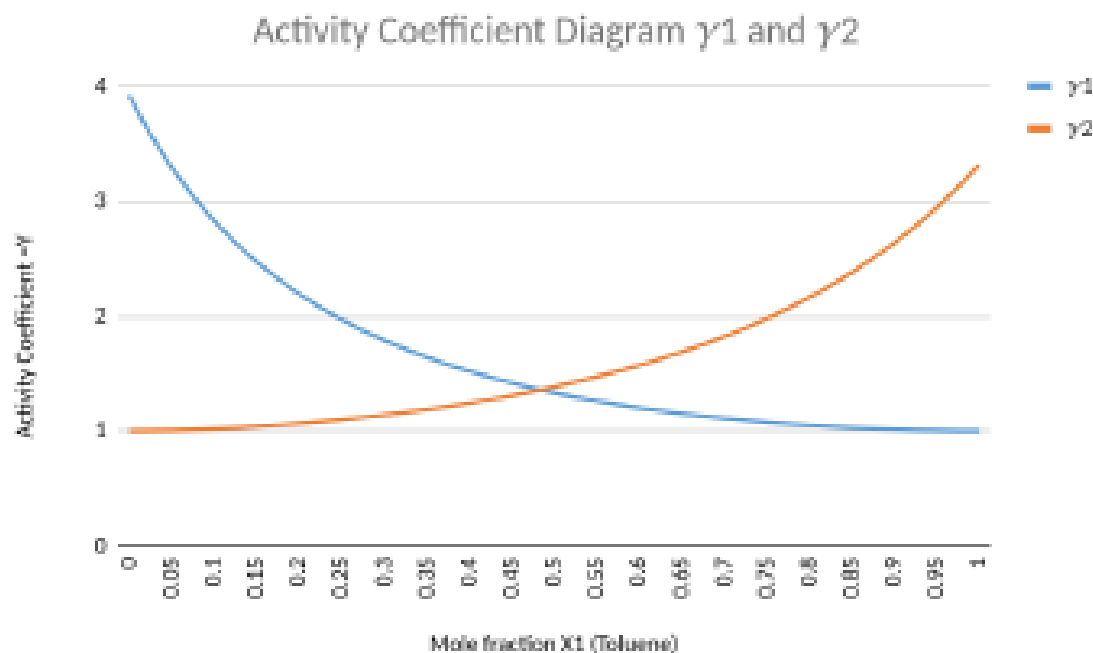
Attached with this letter report, see appendix of Table data showing the values for X and Y found using Wilson, UNIFAC and Peng Robinson models. From these data, we generated an excel spreadsheet showing the calculations for γ_1 and γ_2 .

Activity Coefficient Diagram using Wilson Equations

See below the Wilson equations used to plot the Activity Coefficient Diagrams:

$$\ln(\gamma_1) = -\ln(x_1 + \Lambda_{12}x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} \right)$$

$$\ln(\gamma_2) = -\ln(x_2 + \Lambda_{21}x_1) - x_1 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} \right)$$



Activity Coefficient Diagram using Margules Equations

We used the Margules Equations parameters to calculate γ_1 and γ_2 . The values for A_{12} and A_{21} were obtained from the research paper. Refer to attached appendix A.

$$\ln \gamma_1 = (X_2^2) [A_{12} + 2(A_{21} - A_{12})X_1]$$

$$\ln \gamma_2 = (X_1^2) [A_{21} + 2(A_{12} - A_{21})X_2]$$

$$A_{21} = 0.66$$

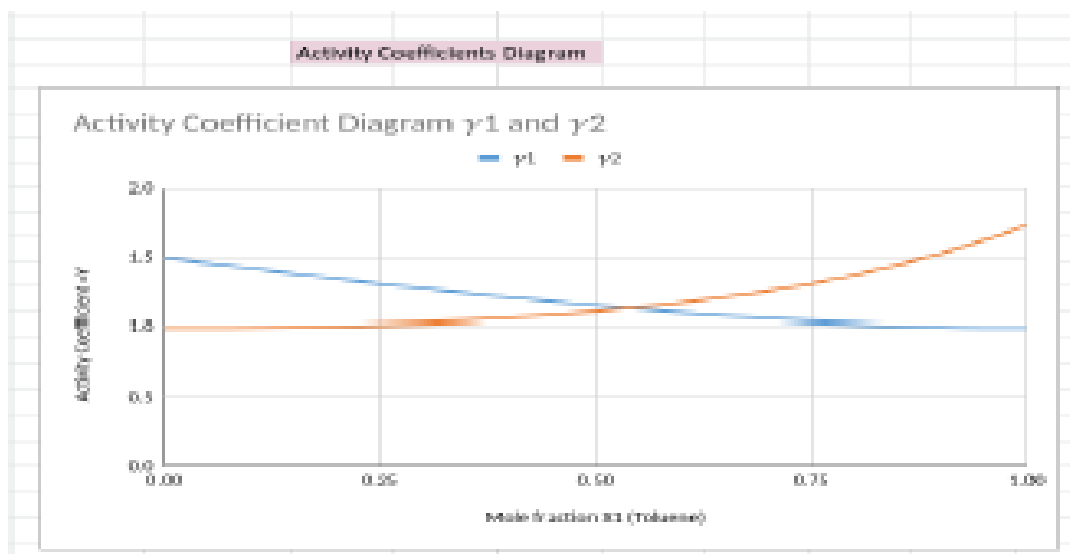
$$A_{12} = 0.4$$

See calculations in excel spreadsheet (Activity Coefficients 1) attached.

Wilson Txy							
X1 (Toluene)	ln γ_1	γ_1	X2 (1-Butanol)	ln γ_2	γ_2	Temperature T	
0	0.4	1.491824	1	0	1	118.156	
0.025	0.3873796875	1.473115	0.975	0.000160	1.00016095	116.606	
0.05	0.3745375	1.454318	0.95	0.000662	1.00066272	115.23	
0.075	0.3615015625	1.435483	0.925	0.001532	1.001533988	114.007	
0.1	0.3483	1.416657	0.9	0.0028	1.002803924	112.919	
0.125	0.3349609375	1.397885	0.875	0.004492	1.004502292	111.95	
0.15	0.3215125	1.379212	0.85	0.006637	1.006639577	111.086	
0.175	0.3079828125	1.360677	0.825	0.009264	1.009307107	110.316	
0.2	0.2944	1.342320	0.8	0.0124	1.012477199	109.628	
0.225	0.2807921875	1.324178	0.775	0.016073	1.01620331	109.013	
0.25	0.2671875	1.306285	0.75	0.020312	1.020520203	108.466	
0.275	0.2536140625	1.288674	0.725	0.025145	1.025464122	107.978	
0.3	0.2401	1.271376	0.7	0.0306	1.031072992	107.546	
0.325	0.226671875	1.254420	0.675	0.036704	1.037306672	107.150	

0.35	0.2133625	1.237833	0.65	0.043487	1.044446939	106.815
0.375	0.2001953125	1.221641	0.625	0.0506976	1.05229823	106.51
0.4	0.1871	1.205868	0.6	0.0592	1.060987417	106.241
0.425	0.1744046875	1.190537	0.575	0.068185	1.070564348	106.004
0.45	0.1618375	1.175669	0.55	0.077962	1.081082117	105.796
0.475	0.1495265625	1.161284	0.525	0.088557	1.092597417	105.616
0.5	0.1375	1.147401	0.5	0.1	1.105170918	105.46
0.525	0.1257853125	1.134059	0.475	0.112317	1.118867695	105.326
0.55	0.1144125	1.121214	0.45	0.125337	1.133757684	105.215
0.575	0.1034078125	1.108943	0.425	0.139689	1.149916191	105.123
0.6	0.0928	1.097242	0.4	0.1548	1.167434453	105.051
0.625	0.0826171875	1.086125	0.375	0.170898	1.186370252	104.999
0.65	0.0728875	1.075609	0.35	0.1889012	1.206848601	104.966
0.675	0.0636390625	1.065707	0.325	0.208170	1.228962494	104.955
0.7	0.0549	1.056434	0.3	0.2254	1.252823745	104.962
0.725	0.0466984375	1.047805	0.275	0.245729	1.278553918	104.995
0.75	0.0390625	1.039835	0.25	0.267187	1.306285352	105.056
0.775	0.0320203125	1.032538	0.225	0.289801	1.336162317	105.149
0.8	0.0256	1.025930	0.2	0.3136	1.36834229	105.281
0.825	0.0198296875	1.020027	0.175	0.338610	1.402997385	105.462
0.85	0.0147275	1.014946	0.15	0.364862	1.440215951	105.705
0.875	0.0103515625	1.010405	0.125	0.392382	1.480504359	106.03
0.9	0.0067	1.006722	0.1	0.4212	1.523789006	106.462
0.925	0.0038109375	1.003818	0.075	0.451342	1.570418568	107.039
0.95	0.0017125	1.001713	0.05	0.482837	1.620666525	107.818
0.975	0.0004328125	1.000432	0.025	0.515714	1.674834011	108.89
1	0	1	0	0.55	1.733253018	110.391

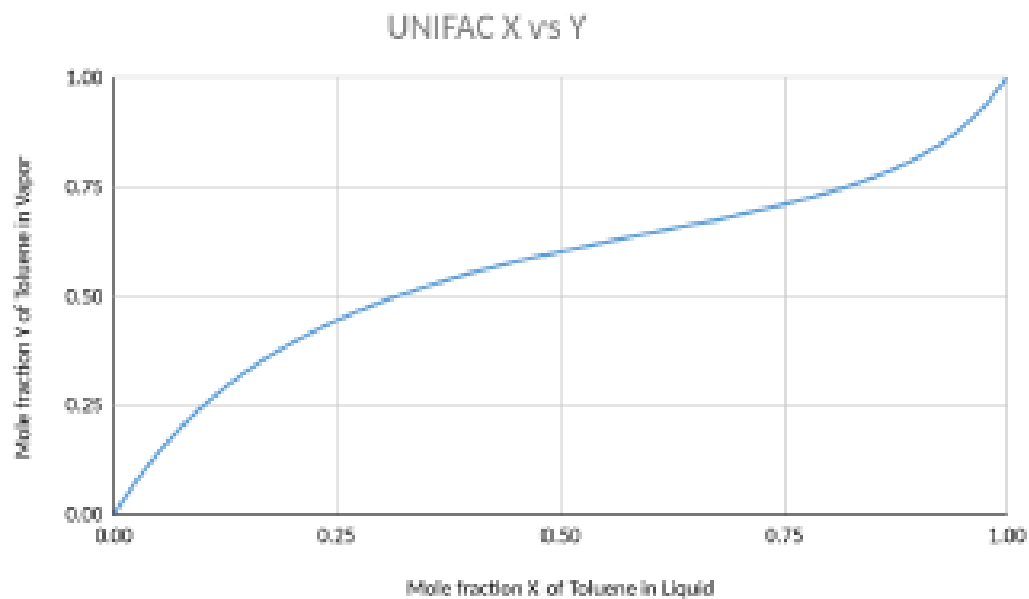
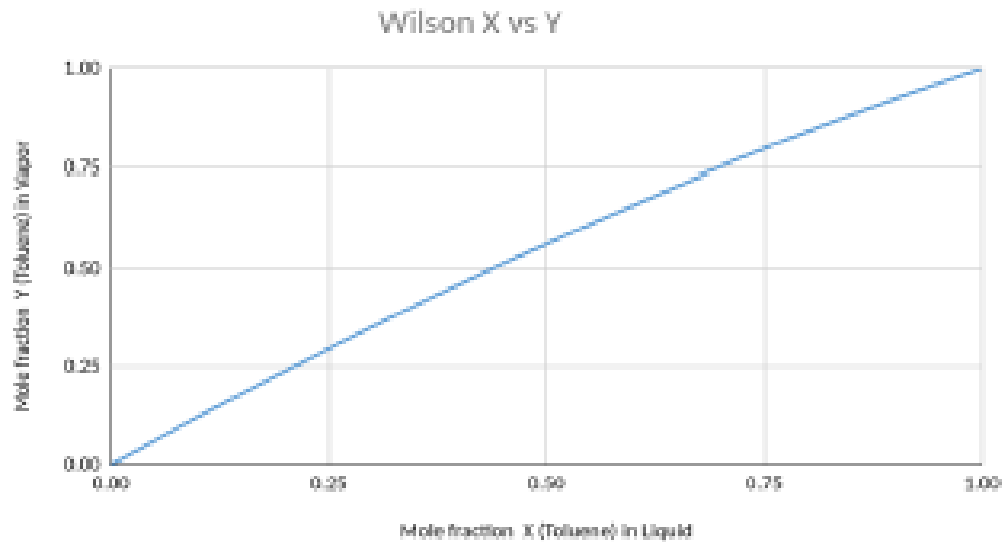
Activity Coefficient graph Calculated from Simulation data



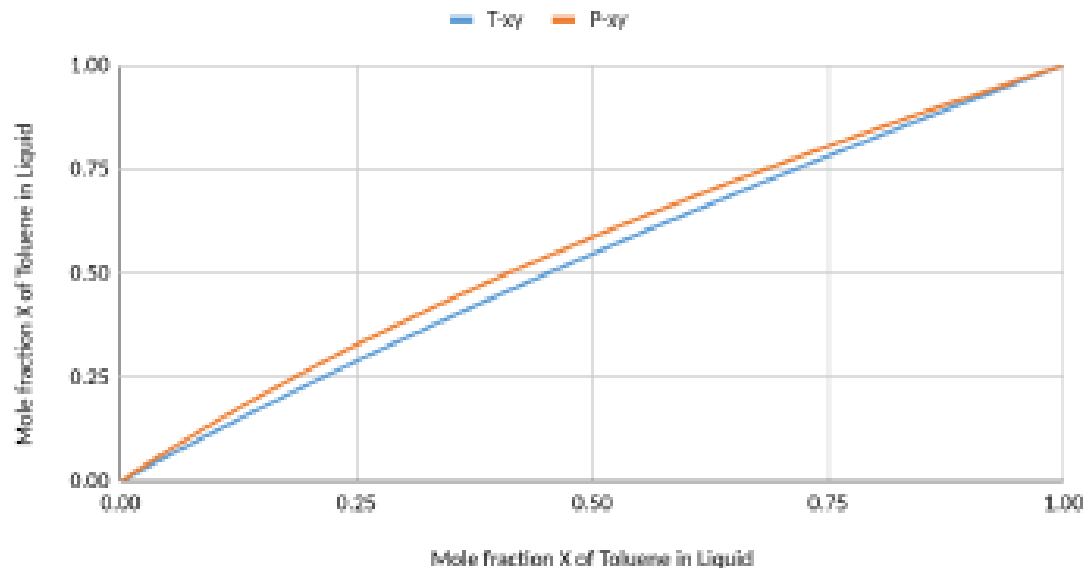
The curve from y_1 goes from roughly 1.5 to 1 and the curve for y_2 goes from 1 to roughly 1.7. Both curves meet roughly at 0.54.

X and Y values obtained from DWSIM Simulation

See attached the "X vs Y values obtained from DWSIM" spreadsheet for the 3 different models. (Wilson, PR and Unifac). See below, graphs obtained from data.



X vs Y graphs using PENG ROBISON model



COMPARISON BETWEEN SIMULATION AND RESEARCH PAPER

T-xy charts

When comparing data from both charts, the research paper shows that T_{sat} for Toluene is 117 °C And T_{sat} for 1-Butanol is 110 °C. Also, the T-xy charts from the DWSIM simulation, for all 3 models, give roughly the same results:

$T_{sat}(1\text{-Butanol}) = 391.2 \text{ K} = 118.05 \text{ °C}$

$T_{sat}(\text{Toluene}) = 383.6 \text{ K} = 110.45 \text{ °C}$

It is important to note that the Wilson model gives a Txy curve that resembles the most to the Txy curve from the research paper.

P-xy Charts

The P-xy charts obtained from DWSIM for all 3 models show that :

$P_{sat}(1\text{-Butanol}) = 34 \text{ KPa}$

$P_{sat}(\text{Toluene}) = 54 \text{ KPa}$

The research paper does not have a representation of the Pxy diagram. However, it is safe to assume that the values for both P_{sat} would be the same or really close.

Activity Coefficients charts

When comparing data from both charts, the research paper shows that the activity coefficient curves meet roughly where X(Mole fraction of Toluene Liquid) is roughly 0.54. The curve from γ_1 goes from roughly 2.5 to 1 and the curve for γ_2 goes from 1 to roughly 3.7. On the other hand, the Activity coefficient chart from the Margules equations shows that both γ_1 and γ_2 curves meet at X= 0.54. However, The curve from γ_1 goes from roughly 1.5 to 1 and the curve for γ_2 goes from 1 to roughly 1.7. From the Wilson equations both γ_1 and γ_2 curves meet at X=

0.50. However, The curve from γ_1 goes from roughly 3.9 to 1 and the curve for γ_2 goes from 1 to roughly 3.3.

X-Y Charts

When comparing the charts, the ones obtained by the DWSIM (Wilson and PR models) and the one obtained from the research paper are similar, with the exception that the chart obtained by the UNIFAC model is more like a concave curve and it is not linear like the other models.

CONCLUSION

The goal of this project was to generate phase diagrams using the DWSIM simulator for Toluene and 1- Butanol mixture, then compare the results obtained to the ones observed in the research papers attached. Both Txy diagrams gave the same results, which were, Tsat (Toluene) was roughly 110 C and Tsat (1- Butanol) was 118 C. The research papers did not show a P-xy Diagram but the P-xy diagrams obtained from the DWSIM simulator (using 3 models) showed that Psat (Toluene) was 54 PKa and Psat (1-Butanol) was 34 PKa. Activity Coefficient diagrams were similar, the curves for γ_1 and γ_2 meet where X (Mole fraction of Toluene in Liquid) = 0.54. However, they also had differences. On the research paper, the Activity Coefficients show that the curve from γ_1 goes from roughly 2.5 to 1 and the curve for γ_2 goes from 1 to roughly 3.7. However, from the Wilson equations both γ_1 and γ_2 curves meet at X= 0.50. However, The curve from γ_1 goes from roughly 3.9 to 1 and the curve for γ_2 goes from 1 to roughly 3.3. the curve from γ_1 goes from roughly 1.5 to 1 and the curve for γ_2 goes from 1 to roughly 1.7. Regarding the X-Y diagrams, they all look similar having a linear shape , except for the Unifac model that had a concave shape.

References

DWSIM Software

Seetharamaswamy, V., et al. "Vapour-Liquid Equilibria for the Systems: Methylcyclohexane-n-Butanol and Toluene-n-Butanol." *Journal of Applied Chemistry*, vol. 19, no. 9, 2007, pp. 258–62. Crossref, <https://doi.org/10.1002/jctb.5010190905>.

Mann, R. S., and L. W. Shemilt. "Vapor-Liquid Equilibria at Atmospheric Pressure. I. 1-Butanol-Toluene System." *Journal of Chemical & Engineering Data*, vol. 8, no. 2, 1963, pp. 189–90. Crossref, <https://doi.org/10.1021/je60017a013>.

AVERAGE

Memorandum

Date: May 2, 2022

To: Dr. Ernest McIntyre

From: Wilfried Zagre

Re: Project 2 – Aspen Simulations of a binary system (CHLOROFORM & BENZENE)

INTRODUCTION:

This project is a study based on the vapor-liquid equilibrium diagram of a binary compound that expresses the bubble point and the dew point of a mixture containing two components referred to as a binary mixture. With the help of ASPEN software, we were able to find a perfect mixture for this thermodynamics project. Basic thermodynamic concepts like the VLE diagram, activity coefficient model selections and the program mentioned previously ASPEN are used in detail throughout the project in order to analyze the binary mixture chosen. Chloroform and Benzene is the binary mixture chosen for this project. The main study was accomplished using the ASPEN plus simulation tool to obtain T-xy diagrams for different local composition models like Van Laar, Uniquac, Unifac, and Wilson. Various quantities like pressure in kPa, mole fraction in mol/mol essentially unitless, Antoine constants: A, B, C and temperature measure.

The figure below shows a T-xy diagram for a binary composition containing chloroform and benzene in the Peng-Robinson local composition model.

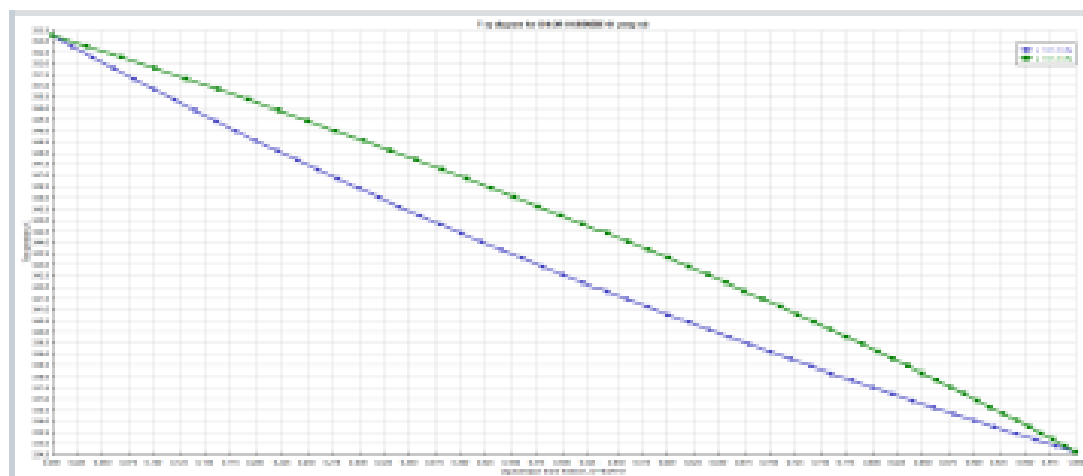


Fig 1.1

CONCEPTS:

All these concepts reviewed in class for VLE will be used in this project.

Binary System: A binary system consists of two components in one mixture. In this case, the components are in vapor and liquid phase. In this project, the binary system will be a mixture of two non-ideal components: chloroform and benzene.

Vapor Liquid Equilibrium: The vapor liquid equilibrium is an important stage when trying to understand the characteristics of a substance between the vapor and liquid phase. Both stages being the extreme side on the graph. By definition the vapor-liquid equilibrium phase is simply defined as the phase where vapor and liquid coexist, both stage in one instant.

Raoult's law: This thermodynamic law states that the partial pressure of each component of a binary mixture is equal to the vapor pressure of the component multiplied by the mole fraction of the mixture. It is represented mathematically by:

$$y_i P = x_i P_i^o$$

The limitation of the Raoult's law is that it only applies to species of known vapor pressure, and this requires each species to be at a temperature below its critical temperature. In other words, Raoult's law only applies to Ideal mixtures. We can overcome this limitation with the use of the modified Raoult's Law.

Modified Raoult's Law: The modified Raoult's law is an extension of the Raoult's law used to solve for non-ideal compositions. In the initial Raoult's law, the values of Gamma and Phi are set to unity or one. Basically, the modified Raoult's law makes adjustment to accommodate the deviation from an ideal solutions behavior. It is mathematically depicted as shown below:

$$y_i P = x_i \gamma_i P_i^o \quad (i = 1, 2, \dots, N)$$

Activity Coefficients: This is symbolically described as gamma γ . The activity coefficient is used to determine the deviation for the ideal state within a binary system.

T-xy Diagram: this diagram clearly shows the relationship between the mole fraction of the liquid and vapor and its corresponding temperature as illustrated in Fig 1.1 above in this case the Pressure is fixed.

P-xy Diagram: Just like the T-xy diagram, the P-xy diagram illustrates the relationship between the mole fraction of liquid and vapor and their corresponding pressure values. and this case the temperature is fixed in both systems the three phases are present but in different location of the graph.

Other concepts that can be used in this project include some composition models like:

1. The Wilson Equation
2. Van Laar Equation
3. Peng Robinson's Equation
4. Antoine's Equation
5. Unifac
6. Uniquac

Wilson Equation: The Wilson's equation is used to determine activity coefficients. It is mathematically denoted as shown below:

$$G^E/RT = -x_1 \ln (x_1 + x_2 \Lambda_{12}) - x_2 \ln (x_2 + x_1 \Lambda_{21})$$

Van Laar Equation: Another well-known equation results when the reciprocal expression $x_1 x_2 RT/G^E$ is expressed as a linear function of x_1 :

$$\frac{x_1 x_2}{\frac{G}{RT}} = A' + B'(x_1 - x_2) = A' + B'(2x_1 - 1)$$

Peng Robinson's Equation: The Peng Robinson equation is expressed mathematically as shown:

$$P = \frac{RT}{V - b} - \frac{a(T)}{(V + \epsilon b)(V + \sigma b)}$$

Antoine's Equation: The Antoine equation is an equation describing the relationship between vapor pressure and temperature for pure substances.

$$\ln P^{sat} = A - \frac{B}{T + C}$$

UNIFAC: UNIFAC is an acronym for Universal quasi-chemical Functional group Activity Coefficients. The UNIFAC model is a common model that uses the functional group of the compound to determine its activity coefficient. It is expressed mathematically as shown below:

$$\ln^i \gamma = \ln^i \gamma^C + \ln^i \gamma^R$$

UNIQUAC: This is an acronym for Universal quasi-chemical Activity Coefficient. It is an activity model used in description of phase equilibrium.

Where:

P- Pressure

x_i - Vapor Phase property (of species i)

R- Gas Constant

P_i^{sat} - Saturated Pressure

V- Molar Volume

T- Absolute Temperature

γ_i – Liquid Phase Property (of species i)

A,B,C - Antoine's constants

Objectives:

The main objectives of this project are listed below:

- Use sources published information such as Perry's Handbook and online sources including the Internet search engines such as Google Scholar, and data base indexes such as Compendex.
- Develop a binary system that does not support Raoult's law with useful VLE data.
- Generate phase diagrams using the ASPEN or DWSIM simulator.

- Select a thermodynamics package to model a binary system.
- Compare simulation results to published data on binary system VLE

While doing the project, all of the objectives set by the professors were met and they will be addressed as you read through....

Results:

For my analyze done during this project, some composition models were employed and they will be shown below as well as the actual values shown in the reference literature.

The table of actual values and T-xy diagram are shown below:

Table 1

T/C	T/K	X	y	P/kPa	A	B	C	P _{sat}	Y	lnY
77.77	350.92	0.142	0.203	101.3	13.7324	2548.74	218.552	169.2113725	0.876	-0.13239
79.49	348.64	0.269	0.373	101.3	13.7324	2548.74	218.552	158.2940856	0.905	-0.09982
74.06	347.21	0.347	0.468	101.3	13.7324	2548.74	218.552	151.728722	0.917	-0.08665
73.28	346.43	0.384	0.513	101.3	13.7324	2548.74	218.552	148.2371792	0.929	-0.07365
72.16	345.31	0.449	0.583	101.3	13.7324	2548.74	218.552	143.3324059	0.932	-0.07042
71.13	344.28	0.496	0.634	101.3	13.7324	2548.74	218.552	138.9332319	0.946	-0.05351
69.28	342.43	0.59	0.73	101.3	13.7324	2548.74	218.552	131.2945066	0.967	-0.03356
67.78	340.93	0.659	0.791	101.3	13.7324	2548.74	218.552	125.3430914	0.981	-0.01918
65.67	338.82	0.768	0.872	101.3	13.7324	2548.74	218.552	117.3279646	0.989	-0.01106
63.9	337.05	0.857	0.928	101.3	13.7324	2548.74	218.552	110.9165689	0.993	-0.00702
62.38	335.53	0.935	0.969	101.3	13.7324	2548.74	218.552	105.6313733	0.999	-0.001

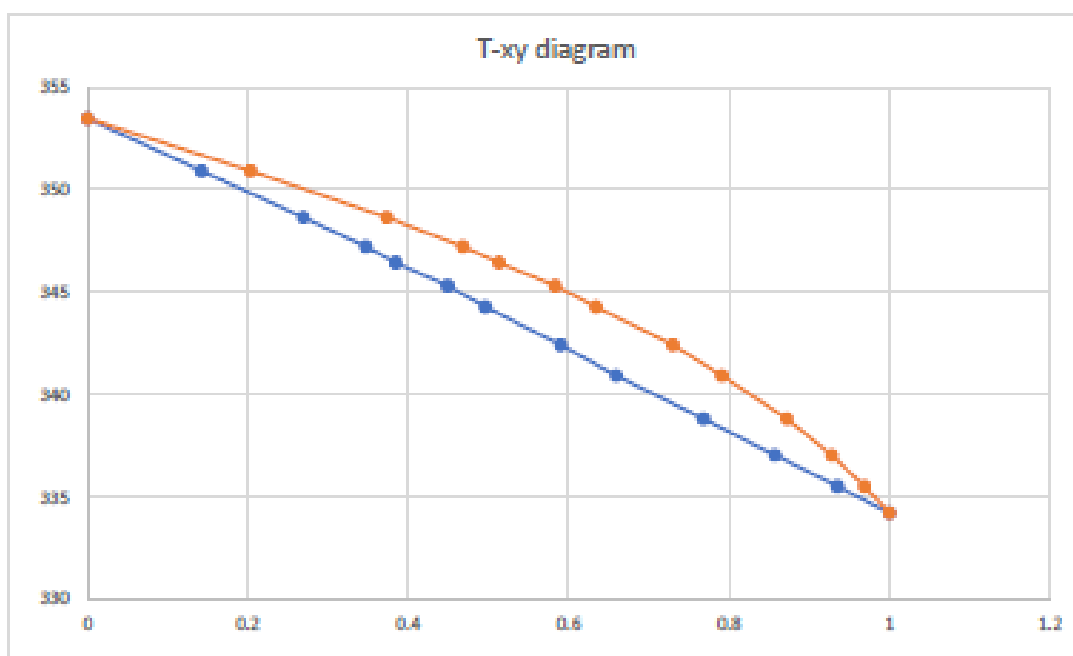
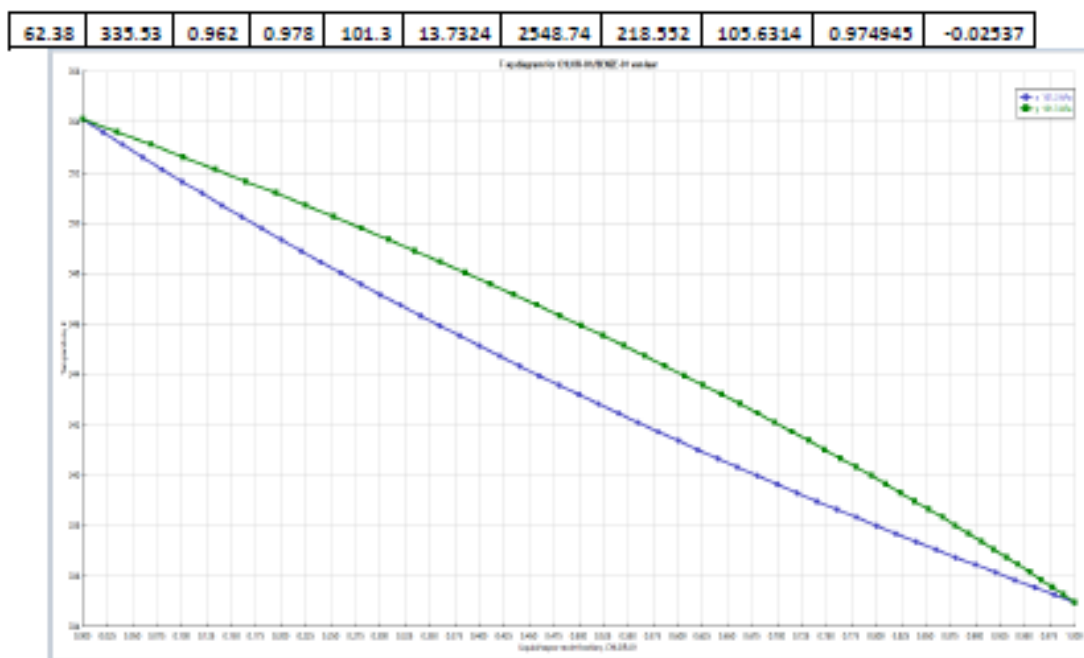


Table of values and T-xy diagram for Van Laar composition model for the chloroform and benzene

Table 2

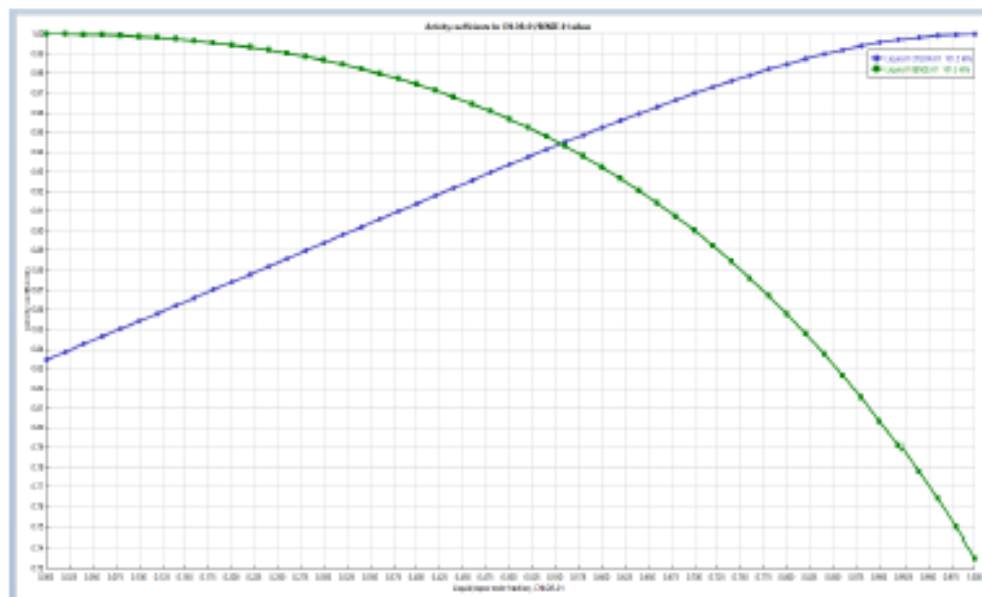
T/C	T/K	x	y	P/kPa	A	B	C	P _{sat}	Y	lnY
77.77	350.92	0.131	0.235	101.3	13.7324	2548.74	218.552	169.2114	1.073931	0.071326
75.49	348.64	0.233	0.35	101.3	13.7324	2548.74	218.552	158.2941	0.961295	-0.03947
74.06	347.21	0.298	0.432	101.3	13.7324	2548.74	218.552	151.7287	0.967832	-0.03268
73.28	346.43	0.335	0.475	101.3	13.7324	2548.74	218.552	148.2372	0.968949	-0.03154
72.16	345.31	0.392	0.537	101.3	13.7324	2548.74	218.552	143.3324	0.968174	-0.03234
71.13	344.28	0.442	0.59	101.3	13.7324	2548.74	218.552	138.9332	0.973269	-0.02709
69.28	342.43	0.542	0.683	101.3	13.7324	2548.74	218.552	131.2945	0.972264	-0.02813
67.78	340.93	0.624	0.752	101.3	13.7324	2548.74	218.552	125.3431	0.973963	-0.02638
65.67	338.82	0.749	0.845	101.3	13.7324	2548.74	218.552	117.328	0.974033	-0.02629
63.9	337.05	0.861	0.918	101.3	13.7324	2548.74	218.552	110.9166	0.973761	-0.02659



For the Wilson model:

Table 3

T/C	T/K	x	y	P/kPa	A	B	C	P _{sat}	$\bar{V}$	$\ln \bar{V}$
77.77	350.92	0.141	0.204	101.3	13.7324	2548.74	218.552	169.2114	0.866146	-0.1437
75.49	348.64	0.269	0.375	101.3	13.7324	2548.74	218.552	158.2941	0.892121	-0.11415
74.06	347.21	0.248	0.47	101.3	13.7324	2548.74	218.552	151.7287	1.265283	0.235296
73.28	346.43	0.388	0.518	101.3	13.7324	2548.74	218.552	148.2372	0.912327	-0.09176
72.16	345.31	0.448	0.586	101.3	13.7324	2548.74	218.552	143.3324	0.924453	-0.07855
71.13	344.28	0.5	0.64	101.3	13.7324	2548.74	218.552	138.9332	0.933283	-0.06905
69.28	342.43	0.592	0.729	101.3	13.7324	2548.74	218.552	131.2945	0.950099	-0.05119
67.78	340.93	0.665	0.795	101.3	13.7324	2548.74	218.552	125.3431	0.966172	-0.03441
65.67	338.82	0.768	0.87	101.3	13.7324	2548.74	218.552	117.328	0.978061	-0.02218
63.9	337.05	0.856	0.93	101.3	13.7324	2548.74	218.552	110.9166	0.992253	-0.00778
62.38	335.53	0.933	0.97	101.3	13.7324	2548.74	218.552	105.6314	0.997026	-0.00298

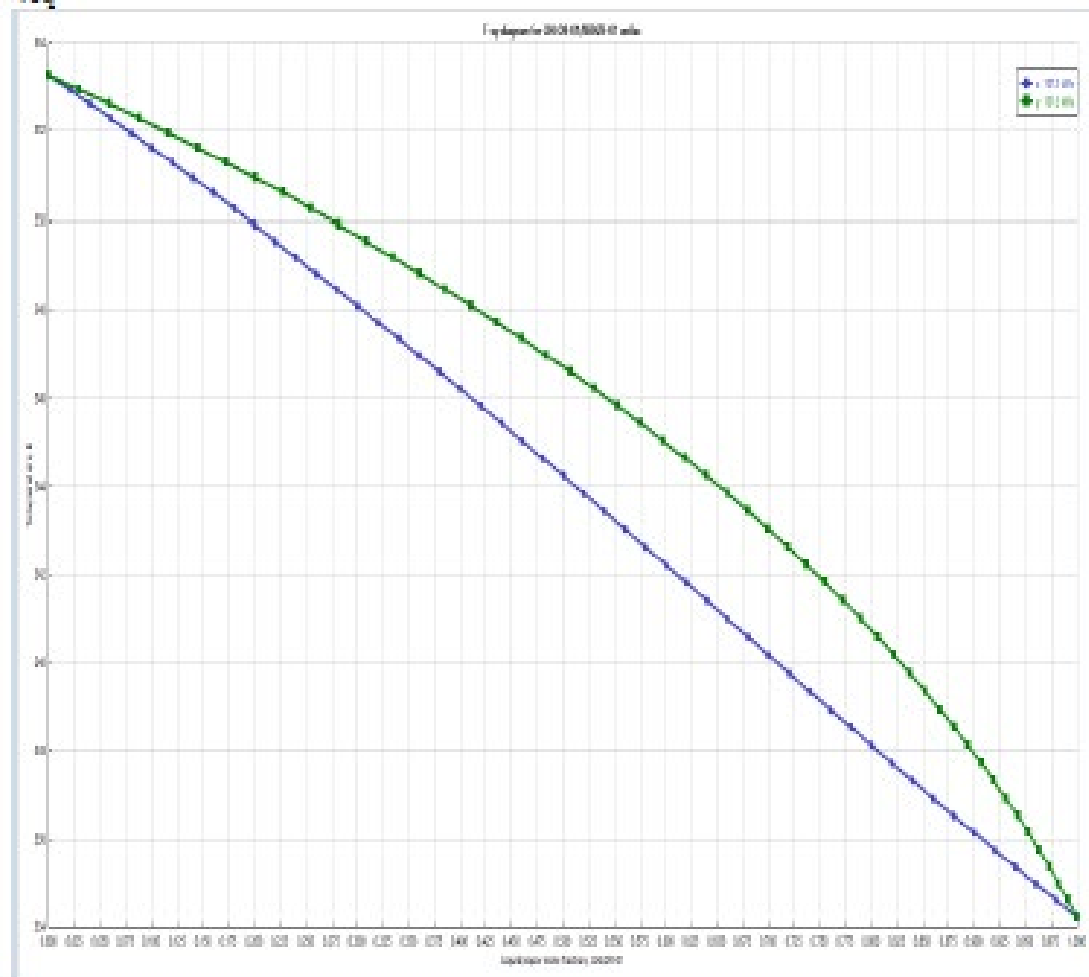


The Unifac model and table of values is as shown below

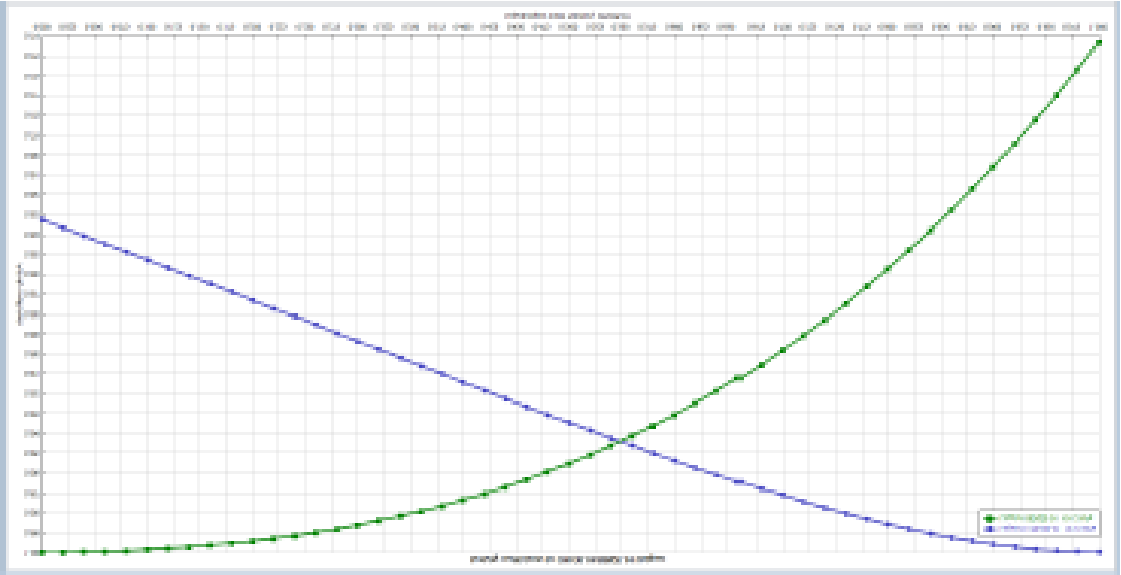
Table 4

T/C	T/K	X	y	P/kPa	A	B	C	Psat	Y	lnY
77.77	350.92	0.141	0.202	101.3	13.7324	2548.74	218.552	169.2114	0.857654	-0.15355
75.49	348.64	0.271	0.375	101.3	13.7324	2548.74	218.552	158.2941	0.885537	-0.12156
74.06	347.21	0.347	0.468	101.3	13.7324	2548.74	218.552	151.7287	0.900447	-0.10486
73.28	346.43	0.389	0.518	101.3	13.7324	2548.74	218.552	148.2372	0.909981	-0.09433
72.16	345.31	0.447	0.582	101.3	13.7324	2548.74	218.552	143.3324	0.920196	-0.08317
71.13	344.28	0.499	0.639	101.3	13.7324	2548.74	218.552	138.9332	0.933692	-0.06861
69.28	342.43	0.59	0.728	101.3	13.7324	2548.74	218.552	131.2945	0.952012	-0.04918
67.78	340.93	0.661	0.792	101.3	13.7324	2548.74	218.552	125.3431	0.968351	-0.03216
65.67	338.82	0.764	0.869	101.3	13.7324	2548.74	218.552	117.328	0.982052	-0.01811
63.9	337.05	0.853	0.927	101.3	13.7324	2548.74	218.552	110.9166	0.99253	-0.0075
62.38	335.53	0.931	0.969	101.3	13.7324	2548.74	218.552	105.6314	0.998138	-0.00186

46q



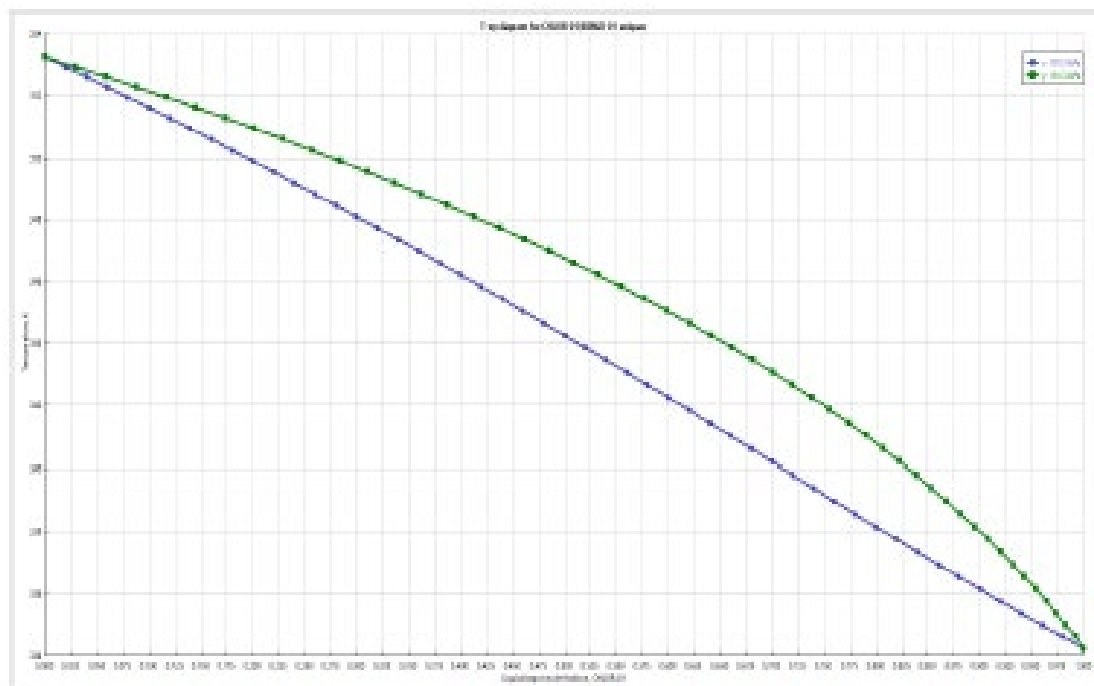
The graph of the activity coefficient against the vapor liquid mole fraction is as shown for Unifac...



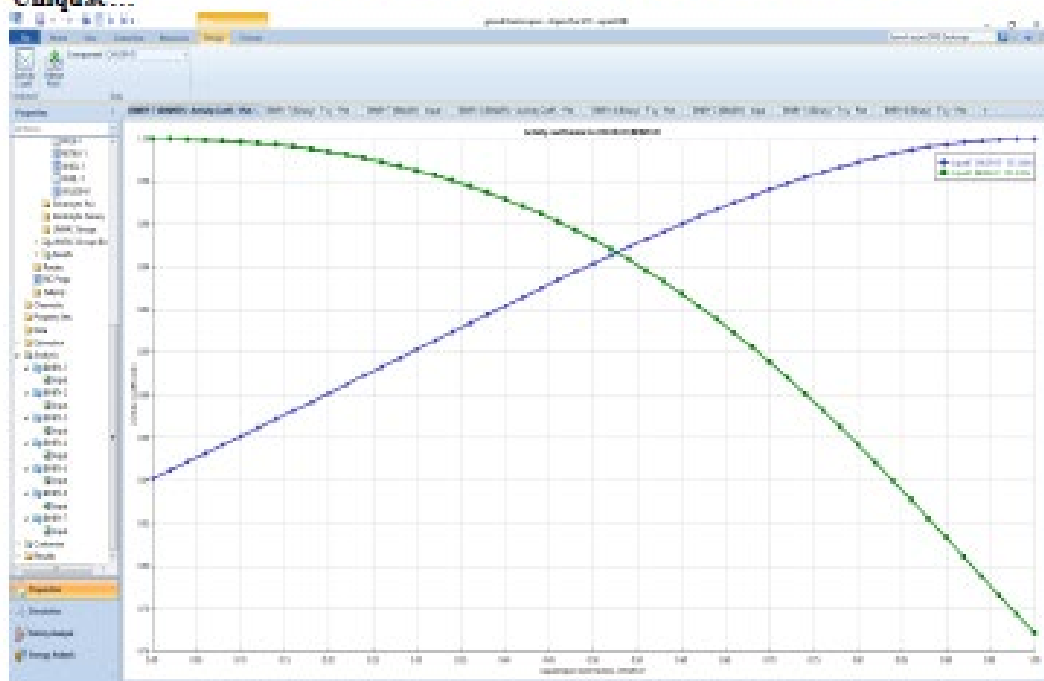
The Uniquac model and table of values is as shown below:

Table 5

T/C	T/K	x	y	P/kPa	A	B	C	P _{sat}	γ	$\ln \gamma$
77.77	350.92	0.14	0.204	101.3	13.7324	2548.74	218.552	169.2114	0.872332	-0.13658
75.49	348.64	0.271	0.376	101.3	13.7324	2548.74	218.552	158.2941	0.887898	-0.1189
74.06	347.21	0.346	0.469	101.3	13.7324	2548.74	218.552	151.7287	0.904979	-0.09984
73.28	346.43	0.4	0.521	101.3	13.7324	2548.74	218.552	148.2372	0.890082	-0.11644
72.16	345.31	0.446	0.584	101.3	13.7324	2548.74	218.552	143.3324	0.925429	-0.0775
71.13	344.28	0.499	0.641	101.3	13.7324	2548.74	218.552	138.9332	0.936614	-0.06548
69.28	342.43	0.59	0.728	101.3	13.7324	2548.74	218.552	131.2945	0.952012	-0.04918
67.78	340.93	0.663	0.794	101.3	13.7324	2548.74	218.552	125.3431	0.967868	-0.03266
65.67	338.82	0.764	0.872	101.3	13.7324	2548.74	218.552	117.328	0.985442	-0.01467
63.9	337.05	0.854	0.929	101.3	13.7324	2548.74	218.552	110.9166	0.993507	-0.00651
62.38	335.53	0.931	0.97	101.3	13.7324	2548.74	218.552	105.6314	0.999168	-0.00083



The graph of the activity coefficient against the vapor liquid mole fraction is as shown for Uniquac...



Discussion: This project is based on the simulation of T-xy diagram for a binary system consisting of Chloroform and Benzene. The local composition models including Wilson, Van Laar, Unifac and Uniquac were used to simulate T-xy diagrams and activity coefficient against the liquid vapor mole fraction with the help of ASPEN. The value of pressure used for all composition models as shown in the various tables is 101.3kPa. The values for saturated pressure P_{sat} were calculated using the Antoine's equation as stated above and the Antoine's constant A, B, C were derived from the recommended book: Introduction to Chemical Engineering Thermodynamics 8th by J.M. Smith, H.C. Van Ness, M.M. Abbott and M.T. Swihart. The values of Temperature, mole fraction of vapor and liquid, x and y, were derived on by using the T-xy diagram.

Conclusion: This report consists of four chosen activity coefficients models which were simulated using ASPEN. Multiple T-xy diagrams were developed for chloroform and benzene and excel sheets and functions to show the variations of VLE diagrams of each activity coefficient in reference to the experimental data. The local models that were employed include the Wilson equation, Van Laar equation, Uniquac and the Unifac models. The VLE diagram that was employed while using the ASPEN plus system in order to derive the activity coefficient graphs. Also, by completing this project our experience with aspen has increased dramatically with generating systems issuing different property methods

BELOW AVERAGE

Memorandum

Date: May 2, 2022

To: Dr. McIntyre

From: Hillary Ndongo

Re: Project 2 – DWSIM Simulations of a binary system consisting of Toluene and Butanol

Objectives:

The main objectives of this project are listed below:

- Use sources published information such as Perry's Handbook and online sources including the Internet search engines such as Google Scholar, and data base indexes such as Compendex.
- Develop a binary system that is not ideal with useful VLE data.
- Generate phase diagrams using the DWSIM simulator.
- Select a thermodynamics package to model a binary system.
- Compare simulation results to published data on binary system VLE

INTRODUCTION:

The project centers around the vapor-liquid equilibrium diagram which is used to express the bubble point and the dew point of a mixture containing two components mostly referred to as a binary mixture. Basic thermodynamic concepts like the VLE diagram, activity coefficient model selections and programs like DWSIM were employed throughout the project to analyze the binary mixture consisting of Toluene and butanol. This project was accomplished using the DWSIM simulation tool to obtain T-xy diagrams for different local composition models like UNIFAC, and Wilson and Peng Robinson. Various quantities like pressure in kPa, mole fraction in mol/mol essentially unitless, Antoine constants: A, B, C and temperature measure in Kelvin, K, and Celsius, C.

Table VII									
System: Toluene (1)-o-Dinitro (2)									
(composition on mole-% basis)									
Vapour-liquid equilibrium at 760 mm Hg									
Run no.	Temp., °C Expt.	Temp., °C Calc.	x_1	y_1 Expt.	P_1 Calc.	y_1 Expt.	P_1 Calc.	y_1 Expt.	P_1 Calc.
1.	116.4	116.2	2.1	4.8	6.9	2.413	1.439	0.8872	1.000
2.	112.6	112.3	4.9	11.0	10.7	2.411	2.157	0.8842	1.001
3.	112.7	112.4	8.1	19.9	19.45	2.413	2.221	1.007	1.006
4.	112.9	111.8	12.9	27.4	27.39	2.943	2.927	0.999	1.014
5.	110.9	110.3	18.3	34.6	34.59	1.965	1.996	1.013	1.029
6.	109.4	109.3	22.2	39.0	39.78	1.761	1.901	1.008	1.063
7.	108.4	108.4	29.9	45.0	44.74	1.612	1.945	1.076	1.076
8.	107.9	107.0	41.8	52.8	52.76	1.411	1.424	1.157	1.163
9.	106.7	106.6	47.5	56.7	56.22	1.446	1.128	1.238	1.229
10.	105.6	106.1	58.5	63.2	61.91	1.214	1.189	1.358	1.379
11.	105.7	106.0	69.5	67.6	67.67	1.114	1.106	1.614	1.594
12.	106.6	106.4	78.5	73.5	73.52	1.049	1.053	1.843	1.837
13.	106.4	105.3	87.5	81.2	81.16	1.017	1.007	2.095	2.162
14.	105.8	106.1	91.8	86.1	86.46	1.012	1.007	2.413	2.441
15.	106.3	106.0	95.6	91.6	91.63	1.005	1.001	2.536	2.554
16.	112.2	109.9	98.2	99.1	99.29	1.000	1.000	2.800	2.793

Vapour-liquid equilibrium at 90 °C									
Run no.	Total pressure, mm. Hg Expt.	Total pressure, mm. Hg Calc.	x_1	y_1 Expt.	P_1 Calc.	y_1 Expt.	P_1 Calc.	y_1 Expt.	P_1 Calc.
1.	382	379	1.3	2.0	4.61	2.298	2.473	1.000	1.000
2.	362	361	4.5	15.0	16.62	2.414	2.183	1.009	1.001
3.	351	349	7.2	21.5	21.69	2.296	2.106	1.009	1.003
4.	348	346	11.4	30.8	31.02	2.168	2.182	1.011	1.009
5.	377	373	17.5	39.2	39.91	2.030	2.046	1.043	1.023
6.	404	399	25.4	48.8	46.19	1.903	1.987	1.099	1.043
7.	422	415	38.4	51.0	50.64	1.816	1.779	1.032	1.064
8.	438	431	56.4	56.5	56.61	1.611	1.696	1.131	1.112
9.	453	448	69.0	60.0	60.15	1.479	1.464	1.203	1.086
10.	456	452	47.2	62.0	61.73	1.415	1.416	1.230	1.222
11.	442	440	53.5	64.5	64.31	1.343	1.322	1.319	1.313
12.	468	465	65.4	68.0	68.16	1.202	1.199	1.351	1.350
13.	470	468	69.6	71.4	70.89	1.115	1.102	1.644	1.644
14.	476	467	79.8	73.0	71.29	1.100	1.099	1.696	1.696
15.	464	464	81.8	77.5	77.34	1.015	1.020	2.132	2.046
16.	469	473	99.6	95.0	94.62	1.009	1.015	2.803	2.842
17.	453	475	96.9	91.9	92.28	0.981	1.002	2.286	2.113

Table 1.1

Concepts:

The following are concepts that were employed during this project.

Vapor Liquid Equilibrium: The vapor liquid equilibrium is an essential concept when trying to understand the characteristics of a substance between the vapor and liquid phase. By definition, the vapor-liquid equilibrium phase is simply defined as the phase where vapor and liquid coexist.

Raoult's law: This law states that the partial pressure of each component of a binary mixture is equal to the vapor pressure of the component multiplied by the mole fraction of the mixture. It is represented mathematically by:

$$y_i P = x_i P_i^{\circ}$$

The limitation of the Raoult's law is that it only applies to species of known vapor pressure, and this requires each species to be at a temperature below its critical temperature. In other words, Raoult's law only applies to Ideal mixtures.

Modified Raoult's Law: The modified Raoult's law is an extension of the Raoult's law used to solve for non-ideal compositions. In the ordinary Raoult's law, the values of gamma and phi are set to unity or one. Basically, the modified Raoult's law makes adjustment to accommodate the deviation from an ideal solutions behavior. It is mathematically depicted as shown below:

$$y_i P = x_i \gamma_i P_i^o \quad (i = 1, 2, \dots, N)$$

Activity Coefficients: This is symbolically described as gamma γ . The activity coefficient is used to determine the deviation for the ideal state within a binary system.

Binary System: As the name implies, a binary system consists of two components. In this case, the components are in vapor and liquid phase. In this project, the binary system will be a mixture of two non-ideal components: toluene and butanol.

T-xy Diagram: this diagram properly illustrates the relationship between the mole fraction of the liquid and vapor and its corresponding temperature as illustrated in Fig 1.1 above

P-xy Diagram: Just like the T-xy diagram, the P-xy diagram illustrates the relationship between the mole fraction of liquid and vapor and their corresponding pressure values.

Other concepts that can be used in this project include some composition models like:

1. The Wilson Equation
2. Van Laar Equation
3. Peng Robinson's Equation
4. Antoine's Equation
5. Unifac
6. Uniquac

Wilson Equation: The Wilson's equation is used to determine activity coefficients. It is mathematically denoted as shown below:

$$G^E/RT = -x_1 \ln (x_1 + x_2 \Lambda_{12}) - x_2 \ln (x_2 + x_1 \Lambda_{21})$$

Van Laar Equation: Another well-known equation results when the reciprocal expression x_1x_2RT/G is expressed as a linear function of x_1 :

$$\frac{x_1x_2}{\frac{G}{RT}} = A' + B'(x_1 - x_2) = A' + B'(2x_1 - 1)$$

Peng Robinson's Equation: The Peng Robinson equation is expressed mathematically as shown:

$$P = \frac{RT}{V - b} - \frac{a(T)}{(V + \epsilon b)(V + \sigma b)}$$

Antoine's Equation: The Antoine equation is an equation describing the relationship between vapor pressure and temperature for pure substances.

$$\ln P^{sat} = A - \frac{B}{T + C}$$

UNIFAC: UNIFAC is an acronym for Universal quasi-chemical Functional group Activity Coefficients. The UNIFAC model is a common model that uses the functional group of the compound to determine its activity coefficient. It is expressed mathematically as shown below:

$$\ln^L \gamma = \ln^L \gamma^C + \ln^L \gamma^R$$

UNIQUAC: This is an acronym for Universal quasi-chemical Activity Coefficient. It is an activity model used in description of phase equilibrium.

Where:

P- Pressure

x_i - Vapor Phase property (of species i)

R- Gas Constant

P_i^{sat} - Saturated Pressure

V- Molar Volume

T- Absolute Temperature

γ_i – Liquid Phase Property (of species i)

A,B,C - Antoine's constants

RESULTS:

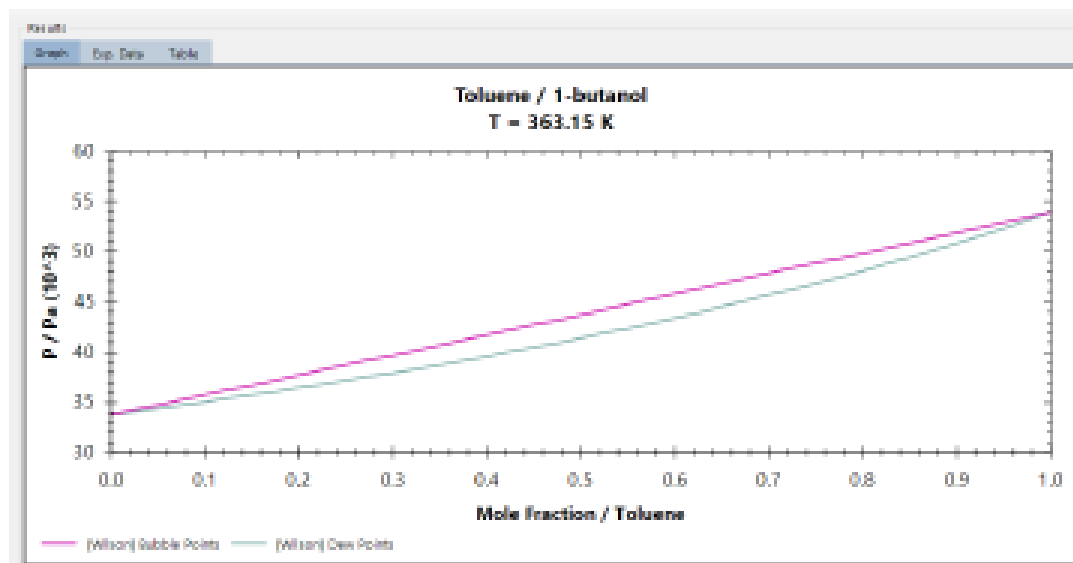
During the process of this project, some composition models were employed, and they will be shown below as well as the actual values shown in the reference literature.

The table of actual values and T-xy diagram are shown below:

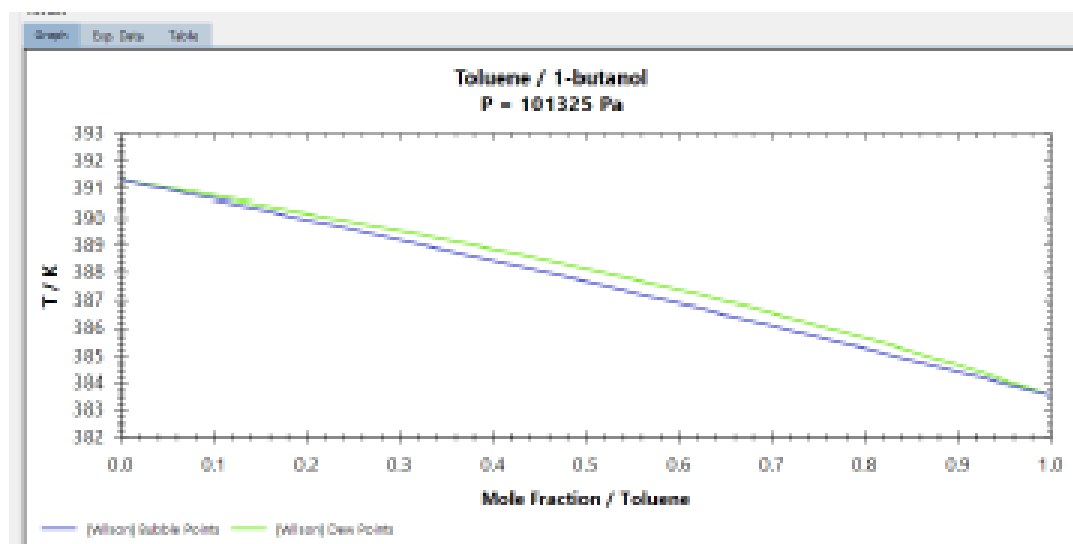
Table 1

T/C	T/K	x	y	P/kPa	A	B	C	P _{sat}	Y	lnY
77.77	350.92	0.142	0.203	101.3	13.7324	2548.74	218.552	169.2113723	0.876	-0.13239
75.49	348.64	0.269	0.373	101.3	13.7324	2548.74	218.552	158.2940856	0.905	-0.09982
74.06	347.21	0.347	0.468	101.3	13.7324	2548.74	218.552	151.728722	0.917	-0.08665
73.28	346.43	0.384	0.513	101.3	13.7324	2548.74	218.552	148.2371792	0.929	-0.07365
72.16	345.31	0.449	0.583	101.3	13.7324	2548.74	218.552	143.3324059	0.932	-0.07042
71.13	344.28	0.496	0.634	101.3	13.7324	2548.74	218.552	138.9332319	0.946	-0.05551
69.28	342.43	0.59	0.73	101.3	13.7324	2548.74	218.552	131.2945066	0.967	-0.03356
67.78	340.93	0.659	0.791	101.3	13.7324	2548.74	218.552	125.3430914	0.981	-0.01918
65.67	338.82	0.768	0.872	101.3	13.7324	2548.74	218.552	117.3279646	0.989	-0.01106
63.9	337.05	0.857	0.928	101.3	13.7324	2548.74	218.552	110.9165689	0.993	-0.00702
62.38	335.53	0.935	0.969	101.3	13.7324	2548.74	218.552	105.6313733	0.999	-0.001

P-xy Wilson

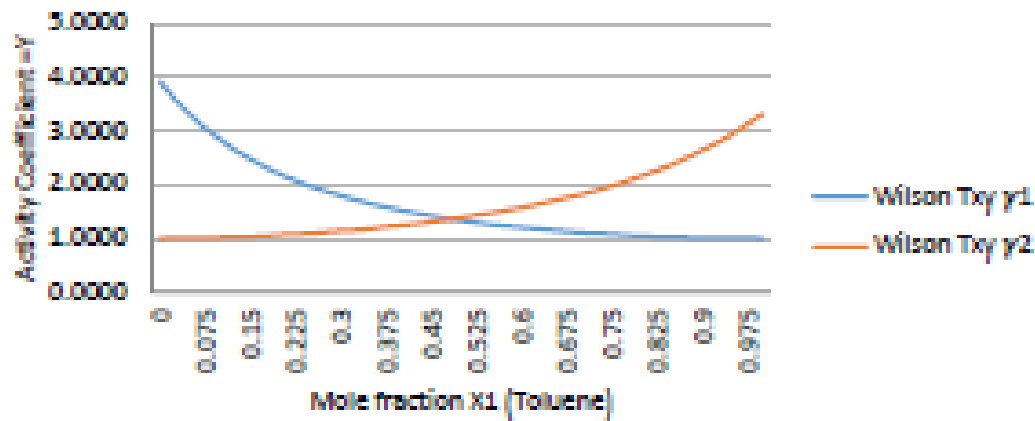


T-xy



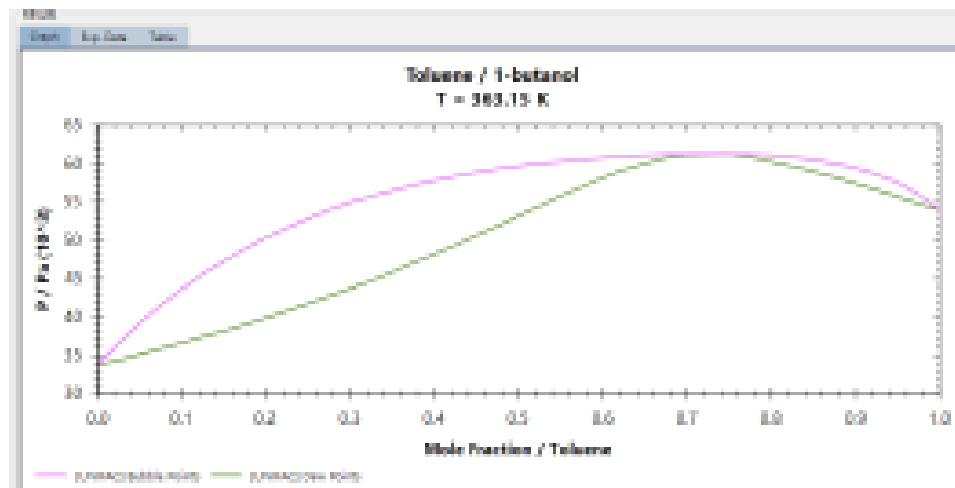
Activity coefficient for Wilson

Activity Coefficient Diagram γ_1 and γ_2

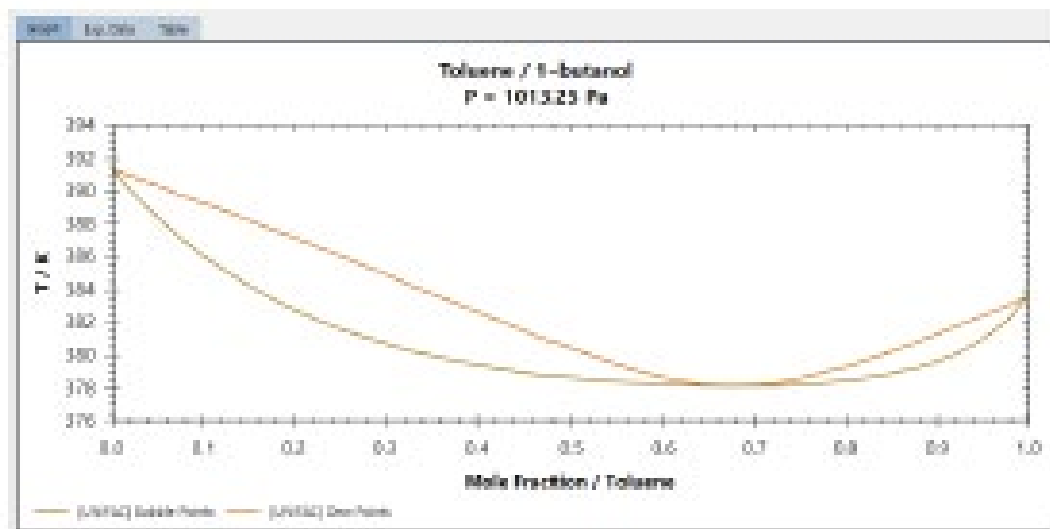


UNIFAC:

T-xy

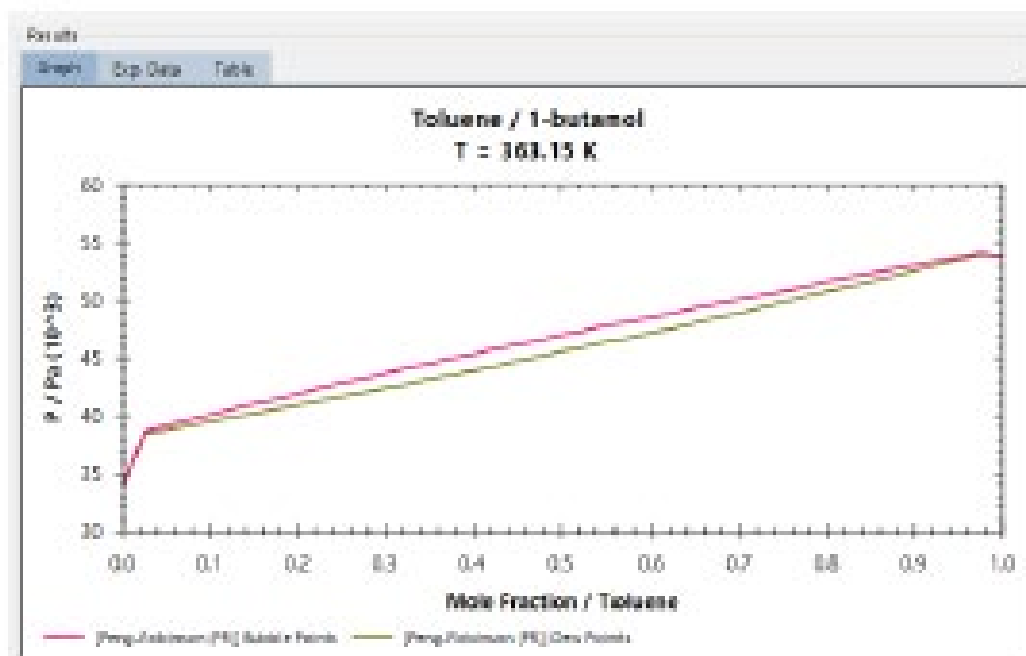


P-xy

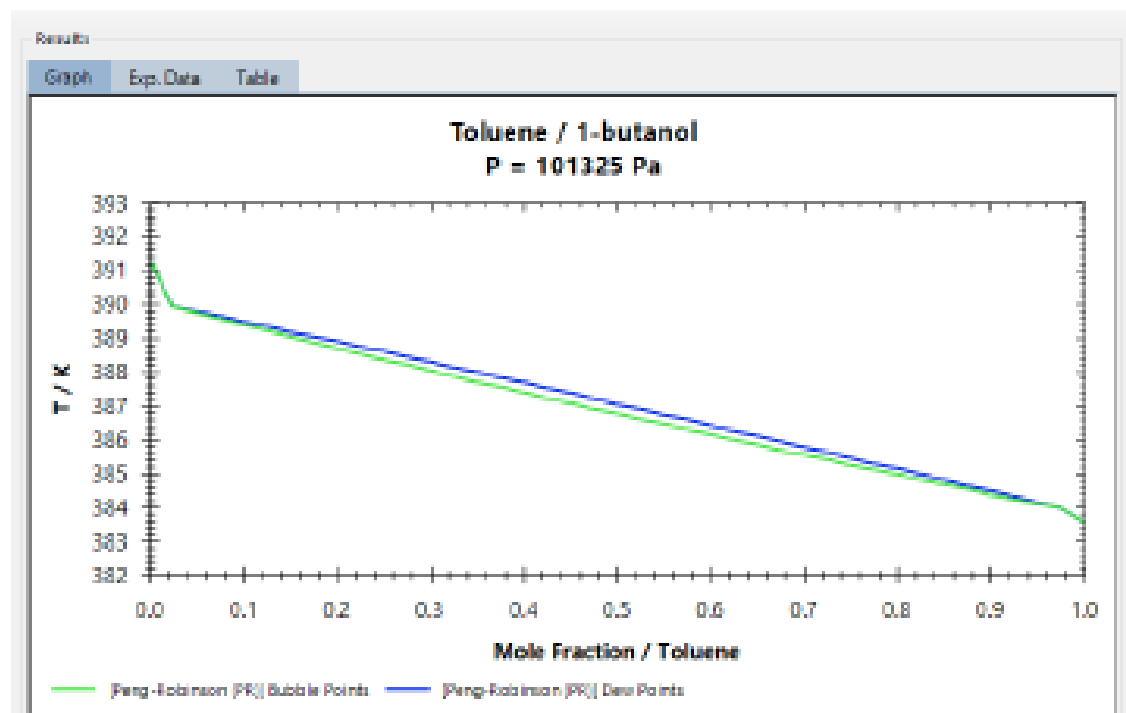


PENG-ROBINSON:

P-xy



T-xy



CALCULATIONS:

This report consists of four chosen activity coefficients models which were simulated using DWSIM. Multiple T-xy diagrams were developed for toluene and butanol and excel sheets and functions to show the variations of VLE diagrams of each activity coefficient in reference to the experimental data. The local models that were used include the Wilson equation, Peng Robinson and the Unifac models. The VLE diagram that was employed while using the DWSIM plus system to derive the activity coefficient graphs. Also, by completing this project our experience with aspen has increased dramatically with generating systems issuing different property methods.

REFERENCES:

- Introduction to Chemical Engineering Thermodynamics 8th by J.M. Smith, H.C. Van Ness, M.M. Abbott and M.T. Swihart
- Activity Coefficients from the Wilson Equation Saral K. Ghosh* and Sawaran J. Chopra Engineers India Limited, New Delhi-110001, india
- DWSIM.

CHEMICAL ENGINEERING THERMODYNAMICS II SPRING 2022

Title of Assignment: UPLOAD VIDEO PRESENTATION FOR PROJECT 1 – Refrigeration Cycle Design Project

TOPICS COVERED IN PROJECT 1

Project 1 covered the following topics:

1. Review of the 1st and 2nd laws of thermodynamics
2. Introduction of refrigeration cycle with application of thermodynamic principles
 - a. Cycles and state properties
 - b. Isothermal, isobaric, reversible, and irreversible processes
 - c. Use of thermodynamic tables
 - d. Real vs. ideal gas behavior
3. Concept of efficiency: compressor efficiency, cycle efficiency and coefficient of performance
4. Phase diagrams (p-H and T-S diagrams) and their use in representing and analyzing a refrigeration cycle
5. Application of 2nd law and concept of approach temperature in selecting condenser & evaporator operating pressure
6. Refrigerant selection based on operating pressure/temperature and global warming potential (GWP)
7. Experience working in teams
8. Oral communication

**CHEMICAL ENGINEERING THERMODYNAMICS II
SPRING 2022**

**SAMPLE ORAL REPORTS SUBMITTED AND
AND GRADING SCHEME FOR PROJECT 1**

ABOVE AVERAGE

Wednesday, October 20, 2021 6:59 AM

Project 1 Refrigeration Cycle Design
September 17, 2021

Criteria (Weight)	4 Expert	3 Proficient	2 Apprentice	1 Novice
Content (30)	Shows a full understanding of the topic. Thoroughly explains and includes readings from the texts, terminology, key questions & answers, and outside research. ✓	Shows a good understanding of the topic. Explains and includes readings from the texts, terminology, key questions & answers, and outside research.	Shows a good understanding of parts of the topic. Explains and includes a small bit of readings from the texts, terminology, key questions & answers, and outside research.	Does not seem to show an understanding of the topic. Little to no explanation; little to no readings from the texts, terminology, key questions & answers, and outside research.
Use of Terms (15) Vocabulary, Pronunciation, Spelling	Uses vocabulary appropriate for the audience and does so correctly. Extends audience vocabulary by defining words that might be new to most of the audience. ✓	Uses vocabulary appropriate for the audience, with some familiarity. Includes some words that may be new to most of the audience and mostly defines them.	Uses vocabulary appropriate for the audience, but is somewhat unfamiliar with some. Does not include any vocabulary that might be new to audience.	Uses several (5 or more) words or phrases that are not understood by the audience, or by the presenter.
Expertise (20) Comprehension of Concepts, Ability to Explain	Student is able to accurately answer almost all questions posed on the topic, such as meaning of terms and importance results. ✓	Student is able to accurately answer most questions posed on the topic, such as meaning of terms and importance results.	Student is able to accurately answer a few questions posed on the topic, such as meaning of terms and importance results.	Student is unable to accurately answer almost all questions posed on the topic, such as meaning of terms and importance results.
Articulation (30) Clarity of Speech, fluency, posture, eye contact	Speaks clearly and distinctly consistently. Stands or sits erect, looks relaxed and confident. Establishes eye and contact during the presentation. ✓	Speaks clearly and distinctly most of the time. Stands or sits erect. Establishes eye contact during the presentation.	Speaks clearly and distinctly much of the time. Sometimes stands or sits erect. Establishes some eye contact.	Mumbles or cannot be understood. Slouches and/or does not look at people during the presentation.
Readiness (10) Level of Preparedness	Student is completely prepared and has obviously rehearsed. ✓	Student seems pretty prepared but might have needed a bit more rehearsal.	Student is somewhat prepared, but rehearsal is clearly lacking.	Student does not seem at all prepared to present.
Teaming (10) Effective interaction of teammates	Excellent ✓	Good	Fair	Poor
Timeliness (5) Punctuality, Use of Time	Presentation began on time and is the correct length. ✓	Presentation began a bit late and/or is nearly the correct length.	Presentation began late or was not the correct length.	Presentation began late and was not the correct length.

Comments:

Refrigeration Cycle Design

- **Compressor**
 - Through an isentropic process vapor is compressed, and a superheated vapor is produced.
- **Condenser**
 - Superheated vapor is condensed a liquid is formed, and liquid is separated.
- **Thermal Expansion Valve**
 - Saturated liquid is expanded through an isenthalpic process, saturated liquid and vapor is produced
- **Evaporator**
 - At constant temperature and pressure liquid is absorbing, saturated liquid is evaporated, and saturated vapor is produced.



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0:37 / 7:48

[illegible]

AVERAGE

Project 1 Team 8 Video Grading

Wednesday, October 20, 2021 6:59 AM

CHEG 3304 CHE Thermodynamics I
Oral Report (Video Articulation)

Project 1 Refrigeration Cycle Design
September 17, 2021

Rubric for Grading Video Presentations for Project 1

Criteria (Weight)	4 Expert	3 Proficient	2 Apprentice	1 Novice
Content (30)	Shows a full understanding of the topic. Thoroughly explains and includes readings from the texts, terminology, key questions & answers, and outside research.	Shows a good understanding of the topic. Explains and includes readings from the texts, terminology, key questions & answers, and outside research.	Shows a good understanding of parts of the topic. Explains and includes a small bit of readings from the texts, terminology, key questions & answers, and outside research.	Does not seem to show an understanding of the topic. Little to no explanation; little to no readings from the texts, terminology, key questions & answers, and outside research.
Use of Terms (15) Vocabulary, Pronunciation, Spelling	Uses vocabulary appropriate for the audience and does so correctly. Extends audience vocabulary by defining words that might be new to most of the audience.	Uses vocabulary appropriate for the audience, with some familiarity. Includes some words that may be new to most of the audience and mostly defines them.	Uses vocabulary appropriate for the audience, but is somewhat unfamiliar with some. Does not include any vocabulary that might be new to audience.	Uses several (5 or more) words or phrases that are not understood by the audience, or by the presenter.
Expertise (20) Comprehension of Concepts, Ability to Explain	Student is able to accurately answer almost all questions posed on the topic, such as meaning of terms and importance results.	Student is able to accurately answer most questions posed on the topic, such as meaning of terms and importance results.	Student is able to accurately answer a few questions posed on the topic, such as meaning of terms and importance results.	Student is unable to accurately answer almost all questions posed on the topic, such as meaning of terms and importance results.
Articulation (10) Clarity of Speech, fluency, posture, eye contact	Speaks clearly and distinctly consistently. Stands or sits erect, looks relaxed and confident. Establishes eye good contact during the presentation.	Speaks clearly and distinctly most of the time. Stands or sits erect. Establishes eye contact during the presentation.	Speaks clearly and distinctly much of the time. Sometimes stands or sits erect. Establishes some eye contact.	Mumbles or cannot be understood. Slouches and/or does not look at people during the presentation.
Readiness (10) Level of Preparedness	Student is completely prepared and has previously rehearsed.	Student seems pretty prepared but might have needed a bit more rehearsal.	Student is somewhat prepared, but rehearsal is clearly lacking.	Student does not seem at all prepared to present.
Teaming (10) Effective interaction of teammates	Excellent	Good	Fair	Poor
Timeliness (5) Punctuality, Use of Time	Presentation began on time and is the correct length.	Presentation began a bit late and/or is nearly the correct length.	Presentation began late or was not the correct length.	Presentation began late and was not the correct length.

Total Score: _____

Comments:

Team 8

- No use of efficiency
- TS diagram shows incorrect cycle 2-3, 3-4
- PH diagram is correct except for 1-2.
- COP given in kW
- Too many sig digs

Carter
Kinsey
Rabb

Team 9

Refrigeration Cycle Design
CHEMICAL ENGINEERING THERMODYNAMICS II - PROJECT 1
Alexis Rabb, Ariel Kinsey, Jaumaine Carter
Submitted a joint submission to the repository of CHEG 3304 Thermodynamics I
Submitted a joint submission to the repository of CHEG 3304 Thermodynamics I

Introduction
The refrigeration cycle is a thermodynamic cycle that transfers heat from a low-temperature reservoir to a high-temperature reservoir. The cycle is used in a wide variety of applications, including air conditioning, refrigeration, and heat pumps.

Project Goals
The goal of this project is to design a refrigeration cycle that meets the following criteria:
1. The cycle must be able to operate at a pressure ratio of 10 or less.
2. The cycle must be able to operate at a temperature ratio of 1.5 or less.
3. The cycle must be able to operate at a COP of 1.5 or less.

Methods
The cycle was designed using the following methods:
1. The cycle was designed using the Rankine cycle model.
2. The cycle was designed using the Carnot cycle model.
3. The cycle was designed using the Otto cycle model.

Results
The results of the cycle design are as follows:
1. The cycle was able to operate at a pressure ratio of 10 or less.
2. The cycle was able to operate at a temperature ratio of 1.5 or less.
3. The cycle was able to operate at a COP of 1.5 or less.

Discussion of Results
The results of the cycle design show that the cycle is able to operate at the required conditions. The cycle is able to operate at a pressure ratio of 10 or less, a temperature ratio of 1.5 or less, and a COP of 1.5 or less. The cycle is able to operate at the required conditions because of the design of the cycle.

Summary
The cycle was designed using the Rankine cycle model, the Carnot cycle model, and the Otto cycle model. The cycle was able to operate at the required conditions because of the design of the cycle.

References
1. Thermodynamics: An Engineering Approach, 8th Edition, Cengel & Boles, McGraw-Hill Education, 2015.
2. Thermodynamics: An Engineering Approach, 7th Edition, Cengel & Boles, McGraw-Hill Education, 2011.
3. Thermodynamics: An Engineering Approach, 6th Edition, Cengel & Boles, McGraw-Hill Education, 2008.

BELOW AVERAGE

Project 1 Team 9 Video Grading

Wednesday, October 20, 2021 6:59 AM

CHEG 3304 **ChE Thermo II**
Oral Report (Video Articulation)

Project 1 Refrigeration Cycle Design
September 17, 2021

Rubric for Grading Video Presentations for Project 1

Criteria (Weight)	4 Expert	3 Proficient	2 Apprentice	1 Novice
Content (30)	Shows a full understanding of the topic. Thoroughly explains and includes readings from the texts, terminology, key questions & answers, and outside research. ✓	Shows a good understanding of the topic. Explains and includes readings from the texts, terminology, key questions & answers, and outside research.	Shows a good understanding of parts of the topic. Explains and includes a small bit of readings from the texts, terminology, key questions & answers, and outside research.	Does not seem to show an understanding of the topic. Little to no explanation; little to no readings from the texts, terminology, key questions & answers, and outside research.
Use of Terms (15) Vocabulary, Pronunciation, Spelling	Uses vocabulary appropriate for the audience and does so correctly. Extends audience vocabulary by defining words that might be new to most of the audience. ✓	Uses vocabulary appropriate for the audience, with some familiarity. Includes some words that may be new to most of the audience and mostly defines them.	Uses vocabulary appropriate for the audience, but is somewhat unfamiliar with some. Does not include any vocabulary that might be new to audience.	Uses several (5 or more) words or phrases that are not understood by the audience, or by the presenter.
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Readiness (10) Level of Preparedness	Student is completely prepared and has obviously rehearsed.	Student seems pretty prepared but might have needed a bit more rehearsal. ✓	Student is somewhat prepared, but rehearsal is clearly lacking.	Student does not seem at all prepared to present.
Teaming (10) Effective interaction of teammates	Excellent	Good ✓	Fair	Poor
Timeliness (5) Punctuality, Use of Time	Presentation began on time and is the correct length. ✓	Presentation began a bit late and/or is nearly the correct length.	Presentation began late or was not the correct length.	Presentation began late and was not the correct length.

Total Score: _____

Comments:

Team 9

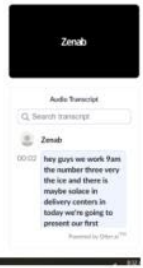
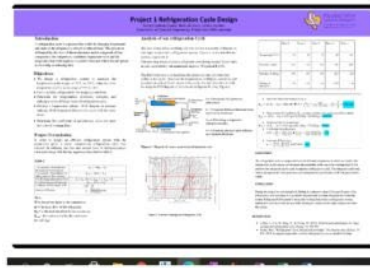
- Used poster style presentation template
- Coulbaly-Diakite
- Did not appear (face not shown) in video
- Contributed most

Salas

- Did not appear (face not shown) in video
- Volume very low

Sanders

- Did not appear (face not shown) in video
- Seemed to be reading a script



CHEMICAL ENGINEERING THERMODYNAMICS II

FALL 2021

**Title of Assignment: UPLOAD ORAL PRESENTATION REPORT FOR
PROJECT 2 – Using ASPEN Simulation for Txy, Pxy Diagram
Generation and Activity Coefficient Model Selection**

TOPICS COVERED IN PROJECT 2

Project 2 covered the following topics:

1. Literature search to find published VLE data for binary systems
2. Ideal solution behavior and departure from Raoult's Law
3. Activity coefficient models accounting for non-ideal solution behavior
4. Generation of phase diagrams (Txy and Pxy) using ASPEN.
5. Comparison of model simulations of phase behavior with real data obtained from the published literature
6. Selection of the best model based on visual observation of overlaid data and theory plots
7. Experience working in teams
8. Oral communication

