University of San Carlos
Department of Chemical Engineering

CHE 4118L Chemical Engineering Laboratory Investigations 2

Data Processing & Analysis Report

(Form CHE 4118L-3)

Prepared and submitted by:

Gibson Jake Canama | Monica Claire Delco | Rhoel Talandron

Experiment : **Distillation of Ethanol-Water in a Batch Distillation Column**

Objectives of the Experiment

1. Determine the average concentration of a specified volume of the distillate that is obtained from a feed mixture of known composition by operating the distillation unit at constant reflux.
2. Use experimental data to predict the time required to obtain a particular concentration of the distillate; and
3. Determine the total number of stages for the batch distillation process.

Results & Discussion

Distillation is the process of selectively boiling and condensation to separate the components or substances in a liquid mixture. It is also a separation process that involves converting a liquid to a vapor, which is then condensed back into a liquid. In several industries, distillation is used to separate liquids from nonvolatile solids, such as alcoholic beverages from fermented materials, or to separate two or more liquids with different boiling points, such as gasoline, kerosene, and lubricating oil from crude oil (Brittanica, 2015).

Distillation is a method of separating the various components of a liquid phase. In both phases, all of the components are present. The vapor phase is formed by vaporization of the liquid phase at the boiling point (Geankoplis, 1993). The composition of the vapor must differ from the composition of the liquid with which it is in equilibrium at the boiling point of the liquid to separate components via distillation. Distillation is concerned with solutions in which all components are appreciably volatile, such as an ethanol-water solution in which both components are vaporized (Geankoplis, 1993).

Rectification (fractionation) or stage distillation with reflux can be thought of as a process in which several flash-vaporization stages are arranged in a series so that the vapor and liquid products from each stage flow counter-current to each other. A stage's liquid is directed or flows to the stage below it, and a stage's vapor flows upward to the stage above it. As a result, a vapor stream and a liquid stream enter each stage, are mixed and equilibrated, and then exit in equilibrium (Geankoplis, 1993).

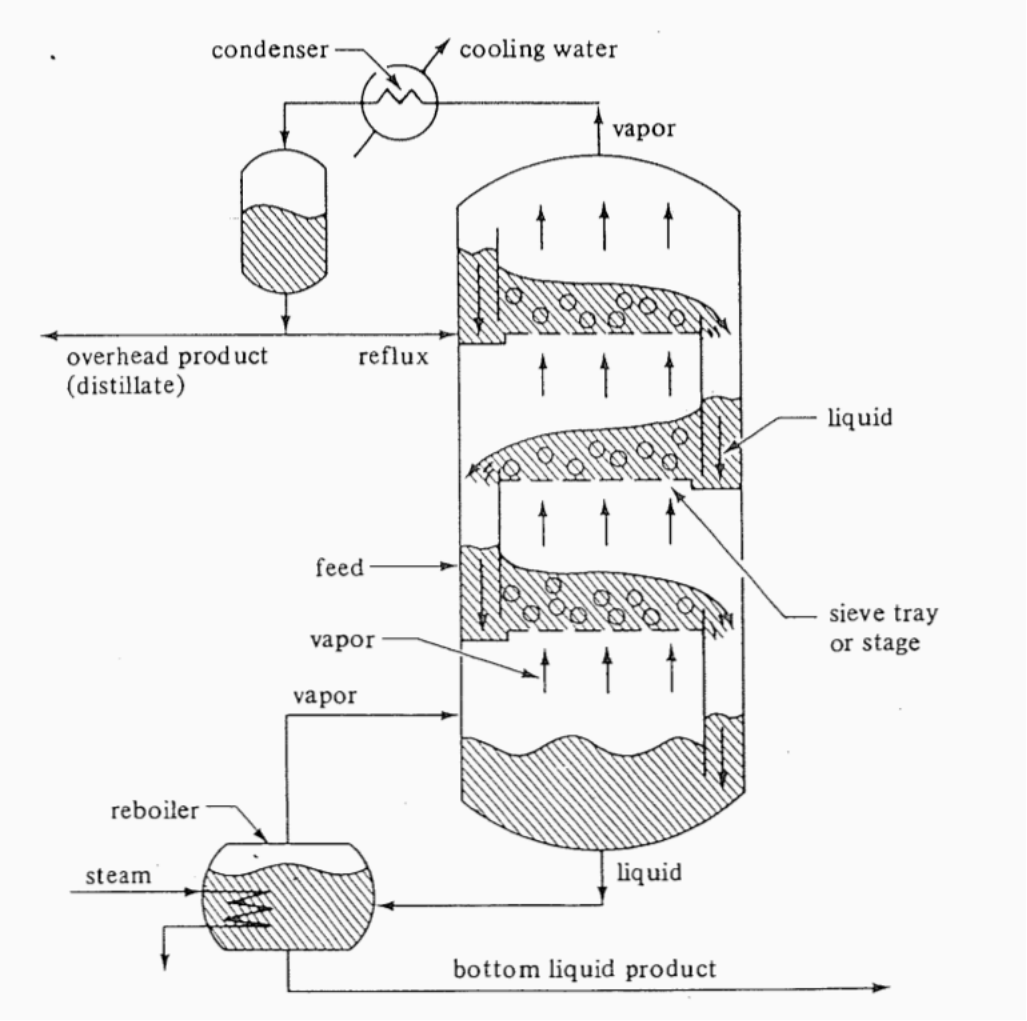

Figure 1. Schematic process flow of a distillation column (Geankoplis, 1993)

The stages in a distillation tower are arranged vertically in a distillation column, as illustrated schematically in Figure 1. The binary mixture being distilled determines the feed entry. The feed flows down to a sieve tray or stage if it is liquid. If the feed is vapor, it enters the tray and bubbles through the liquid as the entering liquid flows across it. The vapor travels to the following tray or stage, where it comes into contact with a down-flowing liquid once more.

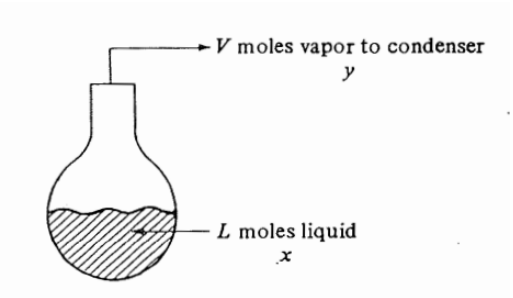

Figure 2. Simple batch or differential distillation (Geankoplis, 1993)

The liquid is initially charged to a heated kettle in simple batch distillation or differential distillation, see Figure 2. The liquid charge is slowly boiled, and the vapors are drawn to a condenser as quickly as they form, where the condensed vapor (distillate) is collected. The more volatile component will be concentrated in the first portion of the condensed vapor. The more volatile component of the vaporized product becomes leaner as vaporization progresses (Geankopolis, 1993). There is no steady-state in batch separations, as the starting charge composition changes with time. As distillation progresses, the still temperature rises, and the relative amount of lower boiler components in the charge decreases.

Through batch distillation of a binary combination of ethanol and water with an initial composition of 30% by weight ethanol, this experiment demonstrates the use of constant reflux to obtain a top product with a specified average composition. A volume of the liquid mixture is charged into the distillation unit, where it is distilled off until a particular volume of distillate is achieved. The mixture is constantly losing its more volatile constituents, and since no new material is added to compensate for the losses, the liquid and vapor concentrations must change continuously throughout the process. The distillation equipment specifications are stipulated in Table 1.

Table 1. Equipment specifications for distillation unit with packed tower (as obtained from the Laboratory Manual)

Equipment specifications	
Reboiler system	Steam heated
Spherical vessel	20-liter nominal capacity
Heat exchanger	Boiler type fitted externally to the spherical vessel in a thermosyphon loop
Fractionating column	Packed tower with manually operated reflux divider
Overhead condenser	Cooling water of inlet temperature of 20 °C and condensation temperature 100°C.
Product Cooler	Generally, gives product temperature less than 10 °C above coolant supply temperature
product receiving vessels	5-liter capacity

A batch distillation with reflux configuration is utilized in this experiment. The more volatile component in the water-ethanol mixture used in the experiment is ethanol. The feed, which contains the mixture to be processed, the ethanol-rich distillate, and the water-rich bottoms make up the system. Figure 3 depicts the setup in diagrammatic form.

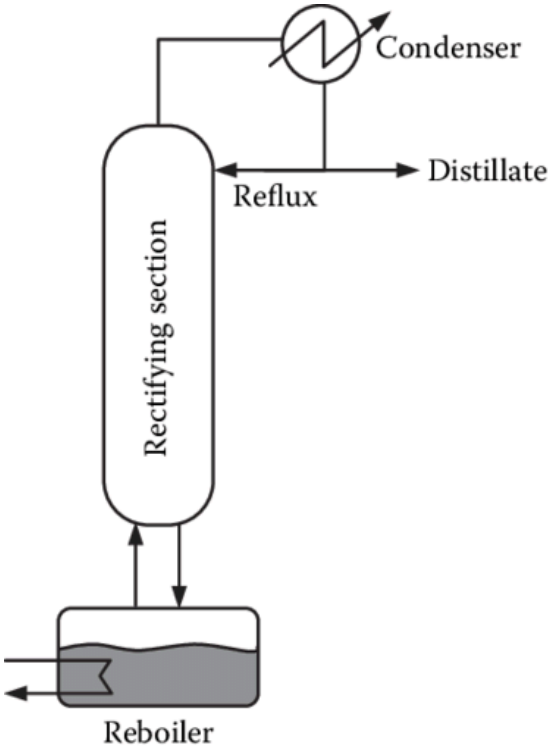

Figure 3. Schematic Diagram of Batch Distillation with Reflux **(Diwekar & Kim, 2005)**

Objective 1: Determine the average concentration of a specified volume of the distillate that is obtained from a feed mixture of known composition by operating the distillation unit at constant reflux

The first objective of the experiment is to determine the average concentration of a specific amount of distillate derived from a known-composition feed mixture by running the distillation unit at constant reflux. The ethanol-water mixture feed was assumed to be prepared at 25^0C at the beginning of the experiment. At an assumed feed temperature of 25^0C, the density of the 30 wt% EtOH solution is 0.951 g/ml. (Engineering ToolBox, 2019). The spherical vessel capacity of the distillation equipment is 20-L as mentioned in Table 1. Hence, the feed volume used was 13.33 L which was 2/3 of the spherical vessel capacity. This feed configuration was done to allocate space for boiling allowance.

Figure 4 shows the composition of the distillate and bottoms as a time series function. The instructor supplied information on the composition of the distillate and bottoms because no actual experiment was undertaken. The y-axis of the graph represents the mole fraction compositions of the

distillate and bottoms, represented by x_D and x_B, respectively. The x-axis is the recorded time in minutes. As seen in the graph, the value of x_D in the distillate increases as time increases. In contrast, the value of x_B at the bottoms decreases with the increase in time. The bottoms' initial and final mole fraction compositions were estimated to be around 0.105 and 0.077, respectively.

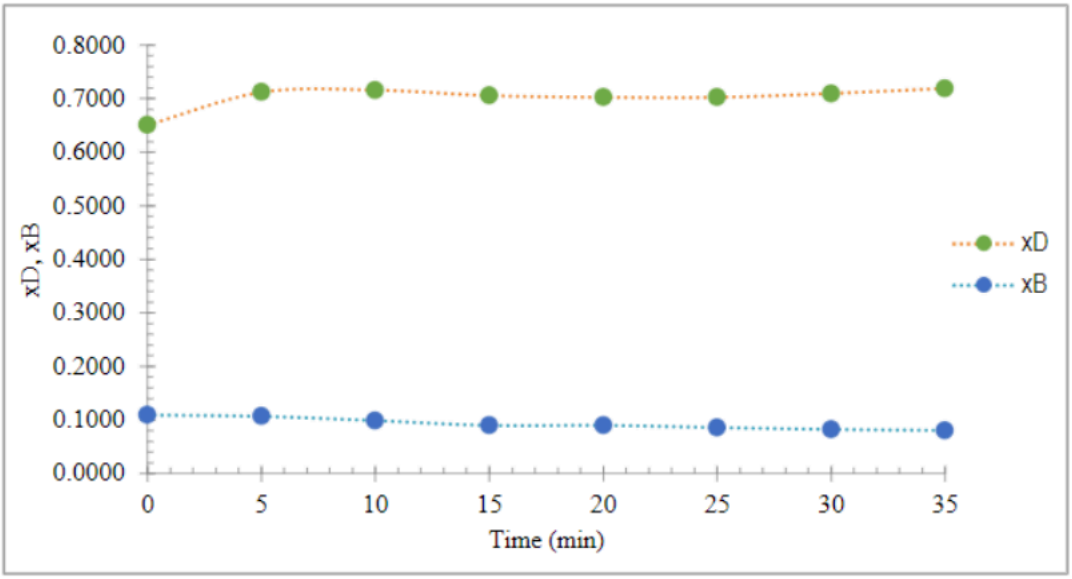

Figure 4. Time series function of the composition of the distillate and bottoms of Ethanol-Water Mixture at an Assumed Feed Temperature of 25^0C @ 101.325 kPa

The determination of the average distillate composition was done theoretically. The initial number of moles in the still was calculated using Equation 1.

$$B_0 = V_{feed} \bullet \rho_{EtOH} \tag{1}$$

where

B_0 = Initial Number of Moles in Still (mol)

V_{feed} = Volume of Feed Mixture Used (13.33 Liters)

ρ_{EtOH} = Density of 30wt% EtOH solution at 25^0C $(0.951 \frac{g}{ml})$

In Figure 2, a simple still is shown. Initially, a charge B_0 moles of the more volatile component (A) and less volatile component with a composition x_{B_0} mole fraction of A is placed in the still. At any given time, there are B moles of liquid left in the still with composition x, and the composition of the vapor leaving in equilibrium is y.

It is important to note that the composition changes with time. In deriving the Rayleigh Equation, it is assumed that only a small amount of dB is vaporized. The composition of the liquid changes from x to $x - dx$ and the amount of liquid changes as well from B to $B - dB$. Hence, generating a material balance on the more volatile component (EtOH) results to

$$Initial\ Amount\ of\ EtOH = Final\ Amount\ of\ EtOH\ in\ Liquid + Final\ Amount\ of\ EtOH\ in\ Vapor$$

Denoting the terms in symbols we have

$$xB = (x - dx)(B - dB) + y\,dB \tag{2}$$

Multiplying out the right side,

$$xB = xB - x\,dB - B\,dx + dx\,dB + y\,dB \tag{3}$$

As stated above, it was assumed that only a small amount of dL is vaporized, hence, the term $dx\,dL$ is neglected. Rearranging,

$$\frac{dB}{B} = \frac{dx}{y-x} \tag{4}$$

Integrating both sides,

$$\int_{B_0}^{B_f} \frac{dB}{B} = \int_{x_{B_0}}^{x_{B_f}} \frac{dx}{y-x} \tag{5}$$

According to Seader et al. (1981), if the reflux ratio is fixed, the distillate and bottoms composition will vary with time and the term $y - x$ in equation 5 is equivalent to $x_D - x_B$ since $y_D = x_D$. Therefore, the final Rayleigh equation is shown in equation 6.

$$\int_{B_0}^{B_f} \frac{dB}{B} = \int_{x_{B_0}}^{x_{B_f}} \frac{dx}{x_D - x_B} \tag{6}$$

where

B_0 = Initial Number of Moles in Still (mol)

B_f = Final Number of Moles in Still (mol)

x_{B_0} = Initial Mole Fraction at the Bottoms

x_{B_f} = Initial Mole Fraction at the Bottoms

A pre-generated plot of $\frac{1}{x_D - x_B}$ against x_B was supplied by the instructor. The plot is shown in Figure 5. The trendline equation of the curve is $y = 71,645x_B^3 - 19,969x_B^2 + 1,848.7x_B - 55.236$ with a correlation value (R^2) of 0.8863.

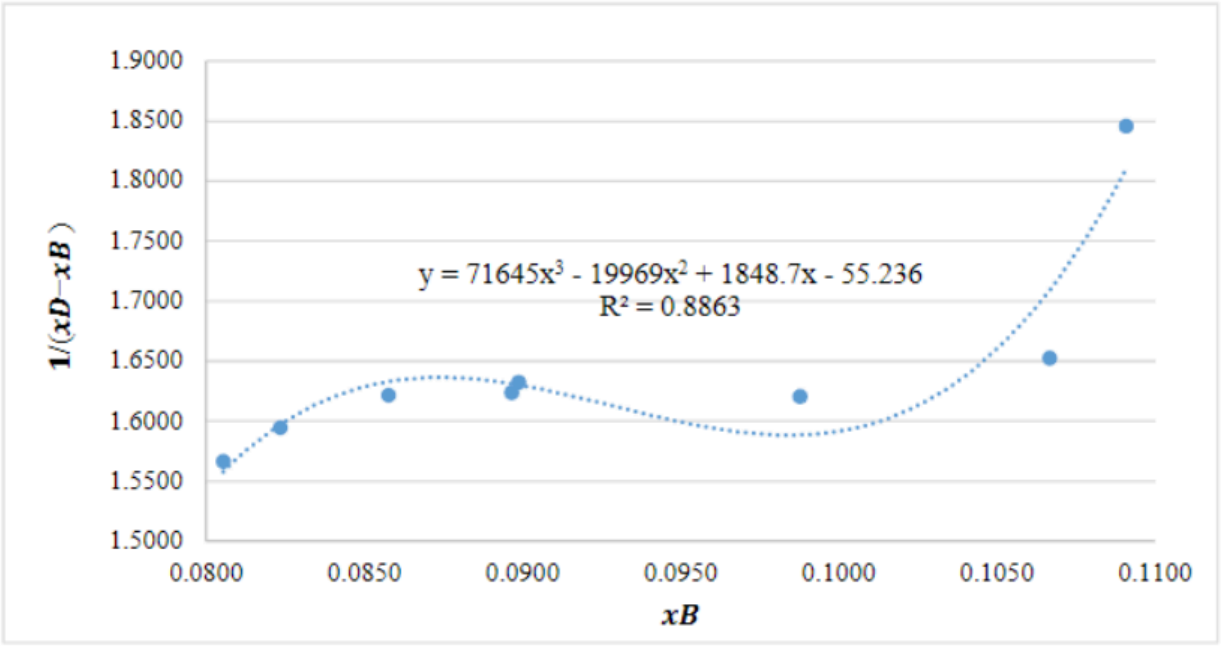

Figure 5. Plot of $\frac{1}{x_D - x_B}$ against x_B for Rayleigh equation of Ethanol-Water Distillation at an Assumed Feed Temperature of 25^{0}C @ 101.325 kPa

As aforementioned, the initial and final compositions at the bottoms were extrapolated from Figure 4. The calculated value of B_0, x_{B_0}, x_{B_f}, and the trendline equation is shown in Figure 5 are then substituted to the Rayleigh Equation to obtain the value of B_f. The analytical integration of the Rayleigh equation resulted to a B_f value of 1114.128 moles.

Furthermore, the average composition of the distillate was calculated using equation 7.

$$x_{D,ave} = \frac{B_0 x_{B_0} - B_f x_{B_f}}{B_0 - B_f} \tag{7}$$

where

$x_{D,ave}$ = Average Distillate Composition (mol/mol)

The average distillate mole fraction composition was calculated to be 0.7180.

Objective 2: Use experimental data to predict the time required to obtain a particular concentration of the distillate

Distillation at 1/6th open reflux valve setting was performed until 3L of distillate was obtained, and the time it took to achieve this was noted. A certain average distillate concentration $x_{D,ave}$ was attained as can be seen in Objective 1. In Objective 2, the predicted or theoretical time to achieve a distillate with such concentration at the same reflux setting is determined.

The reflux was investigated by operating the distillation column under fully open and 1/6th open reflux valve settings. The time elapsed for each reflux setting is stipulated in Table 2.

Table 2. Times to Obtain a Distillate of a Certain Volume at Different Reflux Settings for Ethanol-Water Mixture at Assumed 25˚C and Atmospheric Pressure (101.325 kPa)

Reflux Settings	Time Recorded (mins)
Total Reflux	4.37
1/6 Opening Reflux	9.001

Equation 8 was used to calculate the reflux ratio *R* using a subcooled liquid feed.

$$R = 1 - \frac{t_F}{t_{1/6}} \tag{8}$$

Such that,

t_f = time of distillation at total reflux

$t_{\frac{1}{6}}$ = time of distillation at 1/6 reflux

Meanwhile, the distillate rate D was calculated using Equation 9.

$$D = \frac{\frac{V_D \cdot \rho_{EtOH}}{MW_{EtOH}}}{t_D} \tag{9}$$

Where,

V_D = volume of distillate

ρ_{EtOH} = density of mixture at $x_{D,ave}$

MW_{EtOH} = average molecular weight of mixture at $x_{D,ave}$

t_{pred} = predicted time of distillation

Since the reflux ratio is defined as the ratio of amount of liquid returned to the column *L* to the amount of distillate *D*, *L* was therefore determined using Equation 10.

$$L = RD \tag{10}$$

By mass balance around the column, the boil-up rate *V* can be computed using Equation 11.

$$V = L + D \tag{11}$$

A summary of the results of the calculations above is shown in Table 3.

Table 3. Reflux Ratio, Distillate Rate, Liquid Rate, and Boil-up Rate for the Distillation of Ethanol-Water Mixture at Assumed 25°C and Atmospheric Pressure (101.325 kPa)

Parameter	Value
R	0.5145
D	1.979 mol/min
L	1.018 mol/min
V	2.997 mol/min

The predicted time required for batch distillation can be computed from a total material balance with a constant boil-up rate. The rate at which the feed in the still is expended is equal to the rate at which distillate is produced *D*. Thus, Equation 12 holds true.

$$-\frac{dB}{dt} = D \tag{12}$$

Combining Equation 12 with Equation 11, Equation 13 can be obtained.

$$-\frac{dB}{dt} = V - L \tag{13}$$

Rearranging for integration from time 0 to time *t* and from feed amount B_0 to final amount in the still B_f, we get Equation 14.

$$\int_0^{t_D} dt = -\frac{1}{V-L}\int_{B_0}^{B_f} dB \tag{14}$$

Finally, by integrating and some algebraic manipulation, the predicted time of distillation t_D can be taken using Equation 15. This equation also coincides with that of Seader (2016).

$$t_D = \frac{B_0 - B_f}{V\left(1-\frac{L}{V}\right)} = \frac{(R+1)\left(B_0 - B_f\right)}{V} \tag{15}$$

Table 4 presents the actual t_{act} and calculated predicted t_D times of distillation including the percent error.

Table 4. Actual and Predicted Times of Distillation of Ethanol-Water Mixture at Assumed 25°C and Atmospheric Pressure (101.325 kPa) and its Percent Error

t_{actual} (min)	T_{pred} (min)	% error (%)
35	25.72	36.10

As is presented in Table 4, the percent error (36.10%) can be considered quite large. However, this is expected considering the lack of some relevant data and the subsequent employment of many assumptions (in all objectives) to compensate. One assumption made in the calculations for this objective was that three liters of the distillate were collected as instructed. Another assumption considered is the assumed feed temperature and pressure for the distillation system. These are relevant in determining the distillate rate and othe process parameters.

Objective 3: Determine the total number of stages for the batch distillation process

The design of the distillation setup is described as a fractional column with multiple stages. It is assumed that the tower operates with a feed at atmospheric pressure and room (25°C) temperature. Based on the procedures conducted in the experiment, the separation of a more volatile component (MVC; ethanol) is distilled from the bottoms to obtain a higher concentration of MVC at the receiving end.

It is observed then that the need to address a better separation is to be assessed in the setup is to elevate or maintain the concentration value of the desired product that is to be separated. This can be influenced by the number of stages in the distillation column. According to Tham (2016), the design and performance of the distillation column can be optimized by increasing the number of stages in a column. Thus, we can say that the number of stages of a fractional distillation column does have great importance in the overall performance.

In the experiment, what can be extracted from the raw data are the feed concentration $\left(x_{B_0}\right)$ and the equipment conditions such as temperature and pressure. Further, the calculation of the average distillation concentration $\left(x_{D,ave}\right)$ done in Objective 1 shall be of great use in this objective.

The determination of the relative volatility is based on the ratio of the K-value of the more volatile component to that of the less volatile component (i.e., water). To obtain the value of K of each component, we trace back to the definition which is the ratio of the concentration of component i at vapor phase (distillate) to the concentration of component i at liquid phase (bottoms). With an assumption that the vapor phase is ideal, and the liquid phase is non-ideal and that the pressure is low, we can use a vapor-liquid equilibrium (VLE) relationship in determining K.

$$K_i = \frac{x_{D,i}}{x_{B,i}} = \frac{\gamma_i P_i^{sat}(T)}{P} \tag{16}$$

$$\alpha_{ave} = \frac{K_{EtOH}}{K_{H_2O}} \tag{17}$$

Wherein,

K_i = K value of component i (i.e., EtOH or H_2O)

γ_i = activity coefficient of component i

$P_i^{sat}(T)$ = vapor pressure of component i as a function of temperature T (kPa)

P = pressure (kPa)

α_{ave} = relative volatility of EtOH-water solution

Stipulated in Table 5 are the values of the K-value of each component using UNIFAC Model as the predictive activity coefficient model (Sandler, 2006). The detailed calculations done to obtain K_i and α_{ave} are found in Annex 2 (Processing of Data).

Table 5. Processed Data Values in the Determination of Number of Theoretical Stages for the Distillation of Ethanol-Water Mixture at Assumed Feed Temperature of 25°C and Atmospheric Pressure (P=101.32 kPa)

Parameter	Ethanol	Water
γ_i*	2.9837	1.0255
P_i^{sat}* (kPa)	7.890	3.170
K_i	0.2324	0.0321
α_{ave}	7.2416	
N_{min}	$\approx$ **2**	

*Determined through UNIFAC model software by Sandler (2006).

The Fenske equation is an analytical way of determining the theoretical number of stages at an assumed constant relative volatility. Stipulated in Equation 18, this equation is a rapid estimation of the minimum theoretical stages when the split between components is specified in a binary distillation (Seader, 2016). The influence of the key components in the determination of the theoretical number of stages is reflected on the concentration of each component in the still and the distillate as well as its relative volatility. It can be further inferred that the amount of solution fed in the system is independent of the determination.

$$N_{min} = \frac{\ln ln\left(\frac{x_{D,ave}\left(1-x_{B0}\right)}{x_{B0}\left(1-x_{D,ave}\right)}\right)}{\ln ln\left(\alpha_{ave}\right)} \quad (18)$$

Such that,

N_{min} = minimum number of theoretical stages

From the obtained values of $x_{D,ave}$ and x_{B_0}, the value of N_{min} is acquired based on Equation 18. A more detailed calculation is found in Annex 2 on the calculation of the number of theoretical stages. It was found out that there are applroximately **2 theoretical stages** for the distillation setup. As a basic process parameter for the design of the distillation column, we can say that one can increase the number of stages in the system if we desire more ethanol concentration from the feed and improve its separation (Tham, 2016). Moreover, should one wish to obtain such concentration given the same process conditions, we can use the theoretical stage as the basis of design upon the construction of the distillation column.

Since there is no provided data on the actual number of stages in the distillation set-up, the group cannot deduce the efficiency of the column. However, due to numerous assumptions added to the setup and of the lack of hands-on experience by the members throughout the experiment, we can expect a much higher value of theoretical stages and is much more deviant to the obtained number in this report.

Conclusions

The preparation of the feed mixture was done at room temperature (25^0C). The average distillate composition obtained after batch distillation was calculated to be 0.7180. The time required to obtain a distillate with a certain concentration can be determined from an overall mass balance between the rate of feed depletion and the distillate rate. The predicted time for an average distillate composition of 0.718 was 25.72 min, declaring that the actual distillation time of 35 min exhibits a 36.10% error.

Moreover, the number of theoretical stages of the distillation – using the analytical Fenske Equation – is approximately 2 stages. Errors that may be committed on the processing of data may be rooted in numerous assumptions employed along with the lack of process conditions stipulated on the given group data

References

Brittanica. (2015). *distillation | Definition, Process, & Methods | Britannica*.

Diwekar, U., & Kim, K.-J. (2005). *Batch Distillation*. 107–150. https://doi.org/10.12

Engineering ToolBox. (2019). *Density of Ethanol Water Mixtures*.

Geankoplis, C. (1993). Transport Processes and Unit Operations. Englewood Cliffs, NJ: Prentice-Hall, Inc.

Green, D. W., & Perry, R. (2008). Perry's Chemical Engineer's Handbook. USA: McGraw-Hill Companies, Inc.01/9781420028164.CH5

Sandler, S. (2006). Chemical, Biological, and Engineering Thermodynamics. Hoboken, NJ: John Wiley & Sons, Inc.

Seader, Henley, & Roper. (1981). *Separation Process Principles: Chemical and Biochemical Operations* (Vol. 148).

Wankat, P. (2012). *Separation Process Engineering.* New Jersey: Pearson Education, Inc.

ANNEX 1: Raw Data

Student Performing: Canama

Feed Properties

Volume of Feed (L)	27

Data for Reflux Ratio

Reflux Setting	Time (min)
Total Reflux	4.37
1/6 Reflux	9.001

Molar Compositions of Distillate and of Bottoms at Each Time Interval

Time (min)	Distillate Composition	Bottoms Composition
0	0.6600	0.1100
5	0.7200	0.0950
10	0.7300	0.0900
15	0.7100	0.0850
20	0.7000	0.0800
25	0.7150	0.0800
30	0.7200	0.0750
35	0.7400	0.0750

Temperatures

Setting	Temperature (˚C)
Ambient	25
Boiling Point of 30 wt% EtOH	41.4

Observations

- The observed compositions of still and distillate are of the same range of values; No intense fluctuation nor increase of weight composition of ethanol during distillation operations.
- It takes more time for a distillation under 1/6 opening reflux compared to total reflux given the same collected volume of distillate received.

Student Performing: Delco

Feed Properties

Volume of Feed (L)	27

Data for Reflux Ratio

Reflux Setting	**Time (min)**
Total Reflux	4.37
1/6 Reflux	9.001

Molar Compositions of Distillate and of Bottoms at Each Time Interval

Time (min)	**Distillate Composition**	**Bottoms Composition**
0	0.6500	0.1000
5	0.7100	0.1000
10	0.7100	0.0900
15	0.7000	0.0850
20	0.7000	0.0850
25	0.7000	0.0800
30	0.7050	0.0800
35	0.7200	0.0790

Temperatures

Setting	**Temperature (˚C)**
Ambient	25
Boiling Point of 30 wt% EtOH	41.4

Observations

- Throughout the actual distillation process, the respective bottoms and distillate EtOH compositions do not greatly vary. However, ultimately, the distillation composition increases while the bottoms composition decreases.
- It takes more time to distill at 1/6 reflux than it is at total reflux even with the same distillate volume.
- The boiling point of 30 wt% aqueous EtOH is lower than that of pure water.

Student Performing: Talandron

Feed Composition

Volume of Feed (L)	27
Mass of Feed (kg)	N/A

Times for Distillation

Reflux Setting	**Time (min)**
Total Reflux	4.37
1/6 Reflux	9.001

Compositions of Distillate and of Bottoms at Different Times (every 5 min)

Time (min)	**Distillate Composition**	**Bottoms Composition**
0	0.6500	0.1050
5	0.7150	0.1000
10	0.7100	0.0950
15	0.7000	0.0850
20	0.7000	0.0850
25	0.7050	0.0800
30	0.7075	0.0775
35	0.7200	0.0770

Temperatures

Setting	**Temperature (˚C)**
Ambient	25
Boiling Point of 30 wt% EtOH	41.4

Observations

- As time passes, the obtained composition values of the distillate and bottoms do not show major variances from each data point.
- As time increases, the composition of the distillate also increases. In contrast, as time passes, the bottoms composition decreases
- Distillation with a 1/6 open valve takes longer than distillation with a complete reflux valve.

ANNEX 2: Processing of Data

1. AVERAGE RAW DATA

Time (min)	Distillate Composition			
	TRIAL 1	TRIAL 2	TRIAL 3	AVERAGE
0	0.6600	0.6500	0.6500	**0.6533**
5	0.7200	0.7100	0.7150	**0.7150**
10	0.7300	0.7100	0.7100	**0.7167**
15	0.7100	0.7000	0.7000	**0.7033**
20	0.7000	0.7000	0.7000	**0.7000**
25	0.7150	0.7000	0.7050	**0.7067**
30	0.7200	0.7050	0.7075	**0.7108**
35	0.7400	0.7200	0.7200	**0.7267**

Time (min)	Bottoms Composition			
	TRIAL 1	TRIAL 2	TRIAL 3	AVERAGE
0	0.1100	0.1000	0.1050	**0.1050**
5	0.0950	0.1000	0.1000	**0.0983**
10	0.0900	0.0900	0.0950	**0.0917**
15	0.0850	0.0850	0.0850	**0.0850**
20	0.0800	0.0850	0.0850	**0.0833**
25	0.0800	0.0800	0.0800	**0.0800**
30	0.0750	0.0800	0.0775	**0.0775**
35	0.0750	0.0790	0.0770	**0.0770**

2. OBJECTIVE 1: AVERAGE DISTILLATE CONCENTRATION

Find MW_{EtOH} (30 wt% EtOH) Basis: 100 g mixture

$$mol\ EtOH\ = (30\ g)\left(\frac{1\ mol}{46.07\ g}\right) = 0.65\ mol$$

$$mol\ H_2O\ = (70\ g)\left(\frac{1\ mol}{18.02\ g}\right) = 3.88\ mol$$

$$mol\ mix\ = 0.65\ mol\ +\ 3.88\ mol\ = 4.53\ mol$$

$$MW_{EtOH} = \left(\frac{0.65\ mol\ EtOH}{4.53\ mol\ mix}\right)\left(\frac{46.07\ g\ EtOH}{1\ mol\ EtOH}\right) + \left(\frac{3.88\ mol\ H_2O}{4.53\ mol\ mix}\right)\left(\frac{18.02\ g\ H_2O}{1\ mol\ H_2O}\right)$$

$$MW_{EtOH} = 22.04\ g/mol$$

Find B_0

$$B_0 = V_{feed}\rho_{EtOH} = (13.33\ L)(0.951\ g/mL)\left(\frac{1{,}000\ mL}{1\ L}\right) = 12{,}676.83\ g$$

$$B_0 = (12{,}676.83\ g)\left(\frac{1\ mol}{22.04\ g}\right) = 1{,}165.02\ mol$$

Find B_f

$$\int_{B_0}^{B_f}\frac{dB}{B} = \int_{x_{B0}}^{x_{Bf}}\frac{dx_B}{x_D - x_B}$$

$$\int_{B_0}^{B_f}\frac{dB}{B} = \int_{0.105}^{0.077}\left(71{,}645x_B^3 - 19{,}969x_B^2 + 1{,}848.7x_B - 55.236\right)dx_B$$

$$\ln ln\ B_f\ - \ln ln\ 25{,}677\ g\ = -\ 0.044666$$

$$B_f = 24{,}555.34\ g$$

$$\ln ln\, B_f \; - \; \ln ln\, 1,165.02 \; = - \; 0.044666$$

$$B_f = \; 1114.128\, mol$$

Find $x_{D,ave}$

$$x_{D,ave} = \frac{B_0 x_{B_0} - B_f x_{B_f}}{B_0 - B_f}$$

$$x_{D,ave} = \frac{(1165.02\, mol\,)(0.105) - (1114.128\, mol)(0.077)}{1165.02\, mol - 1114.128\, mol}$$

$$x_{D,ave} = \; 0.7180$$

3. OBJECTIVE 2: PREDICTED DISTILLATE (OPERATING) TIME

Find R

$$R \; = \; 1 \; - \frac{t_{Total\ Reflux}}{t_{\frac{1}{6}\ Reflux}} = \; 1 \; - \frac{4.37\, min}{9.001\, min}$$

$$R \; = \; 0.5145$$

Find MW_{EtOH} ($x_{D,avc}$=0.718)

$$MW_{EtOH} = (0.718\, mol\, EtOH/mol\, mix)\left(\frac{46.07\, g\, EtOH}{1\, mol\, EtOH}\right) + \left(0.282\, mol H_2O/mol\, mix\,\right)\left(\frac{18.02\, g\, H_2O}{1\, mol\, H_2O}\right)$$

$$MW_{EtOH} = \; 38.16\, g/mol$$

Find D

$$D = \frac{V_D \cdot \rho_{EtOH|BP}}{MW_{EtOH}} = \left[\frac{(3L)\left(0.881\ g/cm^3\right)}{(38.16\ g/mol)}\right]\left(\frac{1{,}000\ cm^3}{1\ L}\right) = 69.26\ mol$$

$$D = \frac{69.26\ mol}{35\ min} = 1.979\ mol/min$$

Find L

$$L = RD = (0.5145)(1.979\ mol/min)$$

$$L = 1.018\ mol/min$$

Find V

$$V = L + D = 1.018\ mol/min + 1.979\ mol/min$$

$$V = 2.997\ mol/min$$

Find t

$$t = \frac{B_0 - B_f}{V\left(1 - \frac{L}{V}\right)} = \frac{1{,}165.02\ mol - 1114.128\ mol}{(2.997\ mol/min)\left(1 - \frac{1.018\ mol/min}{2.997\ mol/min}\right)}$$

$$t = 25.72\ min$$

Find %error

$$\%error = \frac{\left|t - t_{act}\right|}{t} \times 100\% = \frac{|25.72\ min - 35\ min|}{25.72\ min} \times 100\%$$

$$\%error = 36.10\%$$

4. Objective 3: Number of Stages in Fractional Batch Distillation

Given:

Feed Composition of MVC $x_{B0} = x_F = 0.1050$

Distillate Concentration of MVC $x_{D,ave} = 0.7180$

Assumptions:

$T = 25℃$

$P = 1\ atm = 101.320\ kPa$

Constant Molar Overflow

(Analytical: Fenske Equation)

At a given temperature T

$$K_{EtOH}(25℃) = \frac{x_{D,EtOH}}{x_{B,EtOH}}$$

Assuming that vapor phase is ideal and liquid phase is non-ideal at low pressure.

$$K_{EtOH}(25℃) = \frac{\gamma_{EtOH} P^{sat}_{EtOH}}{P}$$

Using UNIFAC Model (Sandler, 2006)

$$\gamma_{EtOH} = 2.9837$$

$$P^{sat}_{EtOH} = 7.890\ kPa$$

Therefore,

$$K_{EtOH}(25℃) = \frac{(2.9837)(7.890\ kPa)}{101.320\ kPa}$$

$$K_{EtOH}(25℃) = 0.2324$$

At a given temperature T

$$K_{H_2O}(25℃) = \frac{x_{D,H_2O}}{x_{B,H_2O}}$$

Assuming that vapor phase is ideal and liquid phase is non-ideal at low pressure.

$$K_{H_2O}(25℃) = \frac{\gamma_{H_2O} P^{sat}_{H_2O}}{P}$$

Using UNIFAC Model (Sandler, 2006)

$$\gamma_{H_2O} = 1.0255$$

$$P^{sat}_{H_2O} = 3.170\ kPa$$

Therefore,

$$K_{H_2O}(25℃) = \frac{(1.0255)(3.170\ kPa)}{101.320\ kPa}$$

$$K_{H_2O}(25℃) = 0.0321$$

From the Definition of relative volatility

$$\alpha_{ave} = \frac{K_{EtOH}}{K_{H_2O}}$$

$$\alpha_{ave} = 7.2416$$

Fenske Equation

$$N_{min} = \frac{\ln ln \left(\frac{x_{D,ave}\left(1-x_{B0}\right)}{x_{B0}\left(1-x_{D,ave}\right)} \right)}{\ln ln \left(\alpha_{ave} \right)}$$

$$N_{min} = \frac{\ln ln \left(\frac{(0.7180)(1-0.1050)}{(0.1050)(1-0.7180)} \right)}{\ln ln \left(7.2416 \right)}$$

$$N_{min} = 1.554 \approx 2$$