Modelling, Simulation, and Optimization of Extractive Distillation Columns for the Ethanol Purification Process

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ABSTRACT

Ethanol purification for producing anhydrous ethanol is crucial for internal combustion engine applications. However, separating ethanol from water is challenging due to its azeotropic nature. This study presents a mathematical model and simulation of an extractive distillation column for ethanol purification using MATLAB. The model integrates established methods and equations, including McCabe-Thiele, Lewis Sorel, Fenske's equation, Antoine's equation, Raoult's law, and NRTL thermodynamics. A graphical user interface (GUI) was developed to facilitate user interactions and simulations, mimicking existing chemical engineering process software. The model was validated using Aspen Plus's built-in distillation model. The simulation results showed an optimal reflux ratio of 8, a reboiler duty of 25,725.64 kg/hr, a feed at saturated liquid (q = 1), and an ethanol purity of 99.5%. This condition resulted in minimal reboiler and condenser duties, requiring eight stages for separation. This paves the way for developing indigenous chemical engineering software, reducing reliance on imported software, and supporting industry designers and educational applications in process Engineering. It also emphasizes the importance of integrating modeling and simulation tools to design ethanol purification processes efficiently.

INTRODUCTION

Distillation is a process used to separate components of a mixture based on differences in their volatility. It involves heating the mixture to vaporize the more volatile components and cooling and condensing those vapors into liquid form, separating them from the less volatile components (Seader *et al.,* 2016). In industrial processes, distillation column usage has rapidly increased, and the demand for better control of process conditions has led to greater complications in control mechanisms. Distillation utilizes vapor and liquid phases at the same temperature and pressure for the coexisting zones. Various devices, such as random or structured packings and plates or trays, are used to bring the two phases into intimate contact (Tuan *et al.,* 2016).

Ethanol is a versatile and widely used solvent, fuel, and beverage ingredient in various industries, including the pharmaceutical, chemical, and beverage sectors, and in producing biofuels (Brouwer *et al.,* 2021). Ethanol-water separation is a critical challenge due to the formation of the azeotropic mixture, making conventional distillation ineffective beyond 95.6% ethanol weight composition (Dussier and Sels, 2014). Extractive distillation is a partial vaporization process that enables further separation with the addition of a non-volatile separating agent with a high boiling point, entrainer, or separating agent to the azeotropic mixture to alter the relative volatility of the key component with no additional formation of azeotropes (Gil *et al.,* 2014).

Modeling and simulation are fundamental concepts in chemical engineering that involve creating mathematical representations (models) of real-world processes and systems and then using them to predict or simulate their behavior under different conditions. Engineers can understand, optimize, and design processes without costly experimentation. This can be done using mathematical equations, empirical correlations, or physical laws that govern the system's behavior. Simulation is the execution of a model over time to mimic the behavior of the real-world system. It involves solving mathematical equations or algorithms to generate predictions or simulations of the system's behavior under various conditions (Banks *et al.,* 2005).

The McCabe-Thiele and Lewis Sorel methods are commonly used to determine the number of theoretical plates required for effective separation (Smith *et al*., 2017; Sulayman *et al.,* 2024). These methods use graphical and numerical methods in their separation process to achieve optimal column design. Also, Fenske's equation determines the minimum number of plates necessary for separation (Seader and Henley, 2011). Studies have shown that integrating computational models with thermodynamic principles, such as Antoine's equation and Raoult's law, significantly improves the accuracy of vapor-liquid equilibrium (VLE) predictions (Aspen Technology Inc., 2019).

Phase equilibrium models, such as Non-Random Two-Liquid (NRTL), Universal Quasi-Chemical (UNIQUAC), Wilson models, etc., are essential to describe ethanol-water separation accurately. The Non-Random Two-Liquid (NRTL) model is commonly adopted for polar mixtures because it handles non-ideal interactions between components (Valverde *et al*., 2022). Several studies have compared the performance of NRTL with other thermodynamic models, such as Wilson and UNIQUAC, demonstrating that NRTL provides superior accuracy in predicting VLE behavior for highly polar systems (Gmehling *et al.,* 2010). The NRTL is one of the most common thermodynamic models used in liquid phase calculations because of its capability to produce good calculation results (Hartanto, 2023). Chen et al. (2020) reported a less than 2% deviation in predicted compositions, demonstrating the NRTL model's reliability for ethanol-water separation studies when validated against experimental data.

MATLAB and ASPEN Plus simulation software provide a robust environment for implementing these models due to their extensive mathematical and simulation capabilities. MATLAB, a high-level programming language and interactive environment for numerical computation, provides a flexible environment for implementing numerical algorithms, making it ideal for simulating McCabe-Thiele diagrams and iterative calculations. On the other hand, Aspen Plus, a process simulation software, is widely used for modeling, simulating, and optimizing the behavior of individual unit operations and their interactions within a more extensive process. These tools were chosen for their ability to handle the complex mathematical calculations and simulations required for this study. Zhang *et al.* (2021) simulated an extractive distillation column to achieve 99.5% ethanol purity, validating their experimental results. These outcomes emphasize the importance of integrating modeling and simulation tools to design ethanol purification processes effectively.

METHODOLOGY

Development of the Extractive Distillation Column Model

The extractive distillation column model was developed using MATLAB R2020a software, employing first-principles modeling for steady-state simulation.

Process Description

The extractive distillation process for ethanol-water mixture contains 1-butyl-3-methylimidazolium bromide ionic liquid, which serves as an entrainer by preferentially interacting with water, suppressing its volatility and allowing ethanol to be collected as the distillate. The extractive distillation process model consists of two distillation columns. The first column is the extractive column, where the azeotropic ethanol-water mixture and the entrainer were fed into the column to produce the desired pure ethanol, with the distillate and water as the bottom product. The bottom product (entrainer-water mixture) is passed into the conventional column to separate the entrainer and water. Water is obtained as the distillate while the entrainer is collected as the bottom product and recycled into the extractive column for another separation process (Rojas *et al.,* 2016).

Material Balance Calculation

Mass balances for each stream and component are calculated using the following sets of equations.
Overall material balance:

$$F = D + W \tag{1}$$

Component material balance:

$$x_{fi}F = x_{Di}D + x_{Wi}W \tag{2}$$

where F is the total flow rate of the feed, D is the total flow rate of the distillate, W is the total flow rate of the bottom product. x_{fi} is the mole fraction of each component in the feed, x_{Di} is the mole fraction of each component in the Distillate, x_{Wi} is the mole fraction of each component in the Bottom Product.

Determination of the Number of Theoretical Plates Required for the Separation

The McCabe-Thiele and Lewis-Sorel methods determine the number of theoretical plates needed to separate a distillation column. McCabe Thiele's method employs graphical techniques to determine the number of ideal stages required for a separation in the distillation column. This method involves plotting the equilibrium line, feed line (Equation 3), rectification line (Equation 4), and stripping line (Equation 5) in a y-x diagram. The number of theoretical stages needed for the distillation process is computed through stepwise stage construction between these lines. (Vasconcelos *et al*., 2008).

$$\mathrm{y} = \frac{q}{q-1}x - \frac{z}{q-1} \tag{3}$$

$$\mathrm{y} = \frac{R}{R+1}x - \frac{x_d}{R+1} \tag{4}$$

$$\mathrm{y} = \frac{Lm}{Vm}x - \frac{Bx_b}{Vm} \tag{5}$$

Determination of the Minimum Number of Stages in Each Column

The minimum number of stages (theoretical plates) required for the separation in each distillation column was determined using Fenske's Equation. This equation is beneficial for preliminary design and helps establish a baseline for the number of stages needed under idealized conditions. Equation 6 gives the composition on the first plate for concentrations of two components, **A** and **B**, in the Residue, $x_{Aw,}$ and x_{Bw}.

$$n_{min} + 1 = \frac{\log\left[\left(\frac{x_{Aw}}{x_{Bd}}\right)\left(\frac{x_{Bw}}{xx_{Aw}}\right)\right]}{\log \propto\_AB} \tag{6}$$

where min is the minimum number of theoretical plates in the column, x_{Aw} is the volatility of the highly volatile component at the bottom, x_{Bw} is the volatility of the less volatile component at the bottom, x_{Bd} is the volatility of the less volatile component in the distillate, x_{Aw} is the volatility of the highly volatile component at the bottom.

Determination of the Vapor-Liquid Equilibrium Data

The vapor-liquid equilibrium data of the azeotrope mixture was obtained using Raoult's law and Antoine's equation as described in equation 7. The Antoine equation was used to estimate vapor-liquid equilibrium (VLE) data by incorporating parameters specific to the azeotrope's mixture. It was used to calculate each component's total and partial pressure at different temperatures (Fedali and Madani, 2024).

$$In\ (P_i^s) = A_1 - \frac{A_2}{T+A_3} + A_4T + A_5InT + A_6T^{A_7}, \quad for\ A_8 < A_9 \tag{7}$$

Where T is temperature in K, P_i^s is the vapour pressure component (i) in kPa, A_1-A_9 are the Antoine coefficients specific to component (i). Raoult's Law was used to predict the mole fraction of the component in the distillate and bottom sections of the distillation column. The expression for Raoult's law to be used for the mathematical model is given in equation 8

$$P_a = x_a * P^* \tag{8}$$

where P_a is the component's partial pressure, xa is component A's mole fraction in the liquid phase, and P* is the vapor pressure of the pure component at the given temperature.

Determination of the Minimum Reflux Ratio

Minimum Reflux Ratio calculation provides a benchmark for determining practical reflux ratios in design and operation. Underwood's method for calculating the minimum reflux ratio involves solving equations based on the relative volatilities of the components in the mixture. For a system with components **A** and **B**, the minimum reflux ratio "R_{min}" is calculated using Underwood's equation as shown in equation 9.

$$\frac{\alpha_A\alpha_{dA}}{\alpha_A-\theta} + \frac{\alpha_B\alpha_{dB}}{\alpha_B-\theta} + \frac{\alpha_C\alpha_{dC}}{\alpha_C-\theta} + \cdots \ldots R_m + 1 \tag{9}$$

Where $\alpha_{dA}, \alpha_{dB}, and\ \alpha_{dC}$ are the mole fractions of components A and B. $\alpha_A, \alpha_B\ and\ \alpha_C$ are the volatilities for the least volatile component.

MATLAB Graphical User Interface Development (GUIDE) Method

A graphical user interface (GUI) is a display in one or more windows containing controls, called components, that enable users to perform interactive tasks. The user does not have to create a script or type commands at the command line to accomplish the tasks. Unlike coding programs to accomplish tasks, the user does not need to understand how the tasks are performed (Mathworks, 2015). MATLAB GUI was used to develop a graphical user interface to run the mathematical model.

Validation of model performance

The Aspen Plus V.11 software package was used to validate the performance efficiency correlation developed through MATLAB simulation software. NRTL was selected as the thermodynamic model property due to the nature of the two liquids in the mixture, which are non-ideal and exhibit non-random behavior. The non-ideality condition of the liquid phase was calculated using the Non-Random Two-Liquid (NRTL) method to get the activity coefficient to predict the vapor-liquid equilibrium property, assuming the vapor phase is in the ideal condition. Aspen Plus v11 was used to run the extractive distillation simulation to separate the ethanol-water mixture using 1-butyl-3-methylimidazolium bromide as the entrainer, with input parameters shown in Table 1.

Table 1. Extractive Distillation Column Input Parameters (Hartanto, 2023)

Input Parameter	
Feed (kg/hr)	350
Ethanol Feed mole fraction	0.440
Ethanol Distillate mole fraction	0.974
Residue mole fraction	0.024
Temperature (K)	370
Pressure (atm)	100
Volatility	2.5
Reflux Ratio	3.5

RESULTS AND DISCUSSION

Extractive Mathematical Model

This section explains the extractive distillation model using the ethanol-water mixture's constant and varying input variables. Additionally, the relationship between key parameters, reflux ratio, volatility, and nature of the feed (q) with some fixed parameters like feed and desired ethanol composition, pressure, and temperature were analyzed to determine the number of stages required to achieve the desired separation.

Ethanol-Water Mixture Equilibrium Curve

The equilibrium curve was obtained from the Antoine equation. The extended Antoine equation constant shown in Table 2 was used to model the equilibrium curve shown in Figure 1. It is observed from Figure 1 that the mole fraction of vapor and liquid is 0.45, the ethanol-water mixture was able to attain equilibrium. The Antoine coefficient in Table 2 was used to calculate the saturated pressure for the equilibrium curve plot shown in Figure 2. It is observed from the result of the equilibrium curve that there is interaction between the vapor and liquid phases.

Table 2: The extended Antoine equation constant.

Component	A1	A2	A3	A4	A5	A6	A7	A8	A9
Ethanol	61.7911	-7122.3	0	0	-7.1412	2.88	2	-114	240.85
Water	62.1361	-7258.2	0	0	-7.3037	4.16	2	0.01	373.95
[BMIM][Br]	-1000	0	0	0	0	0	0	0	0

Table 3: Optimum binary interaction parameters for the NRTL model (Merzougui *et al.,* 2012)

Component i	Component j	A_{ij}	A_{ji}	B_{ij} (K)	B_{ji} (K)	C_{ij}
Ethanol	Water	0	0	-34.59	621.73	0.3
Ethanol	[BMIM][Br]	0	0	1089.56	-961.22	0.3
Water	[BMIM][Br]	0	0	2361.08	-1146.1	0.3

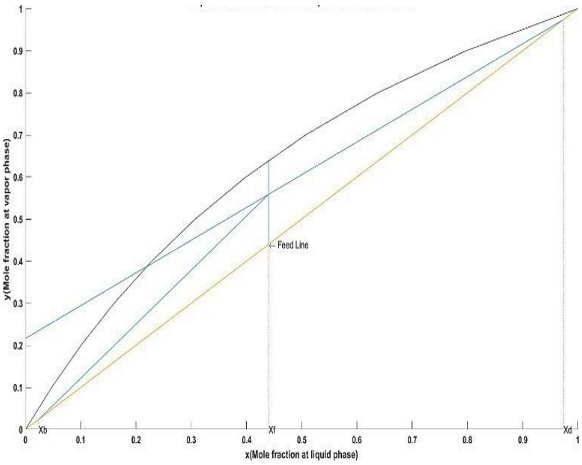


Figure 1: Equilibrium Curve for ethanol-water ideality

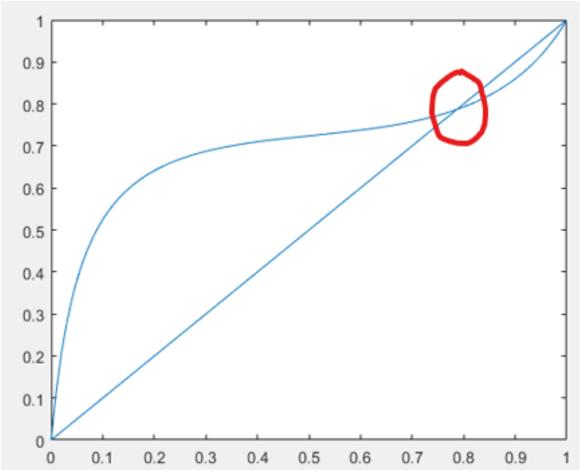


Figure 2: Non-ideality plot in Ethanol-Water-Glycerol Mixture

NRTL Model for Non-Ideality in Ethanol-Water Mixture

The thermodynamic property package, NRTL, was implemented to cater to the non-ideality in the ethanol-water mixture and calculate the activity coefficient. The result of the model is shown in Figure 2, while the input parameters shown in Table 3 were used for its modelling. Figure 2 shows that the red circled point indicates the azeotropic behaviour of the ethanol-water mixture. Figure 3 reveals the effect of introducing the entrainer to break the azeotrope point for further separation, which caters to the non-ideality in the ethanol-water mixture.

WILSON Model for Non-Ideality in Ethanol-Water Mixture

The thermodynamic property package, WILSON, was implemented with input parameters shown in Table 4 to determine which of the two models best fits the extractive distillation process. The model result, Figure 4, indicates that the WILSON model also removes the non-ideality in the ethanol-water mixture by breaking the azeotropic point after introducing the entrainer.

Txy diagram of Ethanol-Water Mixture

The T_{xy} diagram of the ethanol mixture plot with the two thermodynamic models, NRTL and WILSON, Figure 5, shows the relationship between the temperature and liquid composition of the ethanol-water mixture and the azeotropic condition. It is observed that the NRTL model is influenced by temperature variation and its effect on the liquid and vapor phases. The number of stages to achieve the desired composition of 0.97% ethanol at the distillate was determined using the McCabe-Thiele method at saturated liquid for the feed. The result of the effect of the nature of feed (q) on the number of stages, reboiler steam required, and cooling water needed on the number of stages of the distillation column is shown in Table 5.

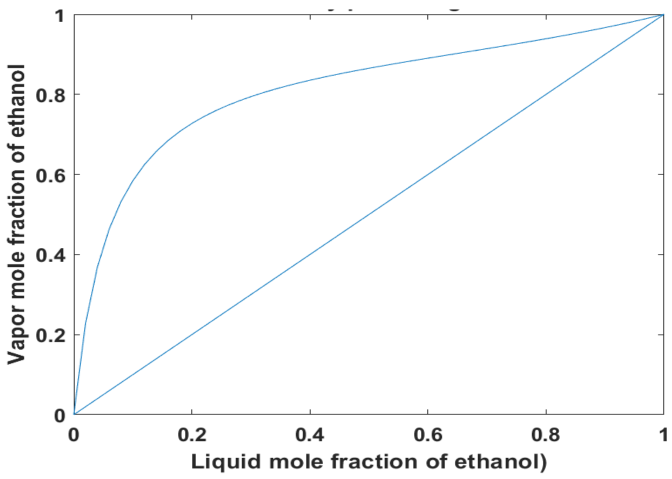
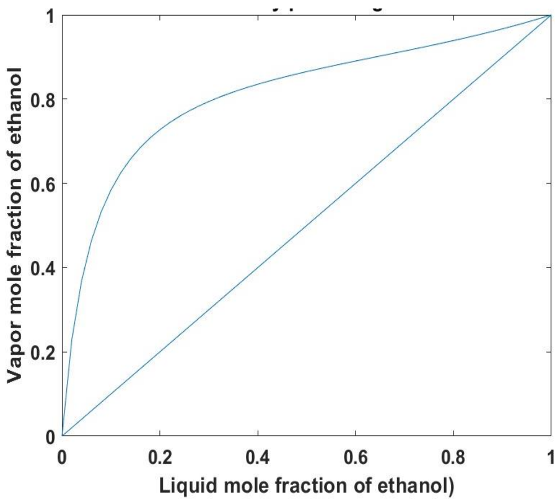


Figure 3: NRTL azeotropic plot of Ethanol-Water-Glycerol Mixture

Table 4. WILSON Binary Parameter for Ethanol-Water-Glycerol

Substances	**Binary Parameters**				
	Aij	**Bij**	**Cij**	**Dij**	**eij**
Ethanol	[0 -2.5035 0]	[0 346.1512 -120.5482]	0	0	0
Water	[-0.050, 0, 0.643]	-69.6372 0 -131.2562]	0	0	0
[BMIM][Br]	[0, 1.1766, 0]	[-400.0392 -264.2581 0]	0	0	0



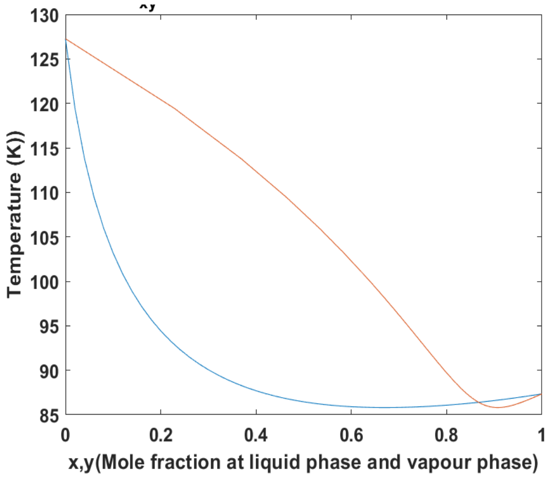


Figure 4: WILSON plot result for non-ideality in Ethanol-water-glycerol mixture

Figure 5: T_xy diagram plot for ethanol-water mixture

It is observed from Table 5 that the higher the value of the nature of the feed, q, that is, the more the nature of the feed gets sub-cooled, the higher the reboiler duty, while the number of stages increased until it reached a point where it became constant. The number of stages remains constant when q=1.5.

Table 5. Effect of nature of feed (q) on the number of stages, reboiler steam required, and cooling water required

q	Number of stages	Steam required (kg/hr)	Cooling water required (kg/hr)
-3	8	-10824	366239.56
-2.5	8	-8155.95	366239.56
-2	7	-5487.37	366239.56
-1.5	6	-2818.79	366239.56
-1	6	-150.2	366239.56
-0.5	8	2518.38	366239.56
0	15	5186.96	366239.56
0.5	11	7855.54	366239.56
1	11	10524.13	366239.56
1.5	10	13192.71	366239.56
2	10	15861.29	366239.56
2.5	10	18529.87	366239.56
3	10	21198.45	366239.56

The effect of the reflux ratio on the number of stages is shown in Table 6. It was observed that the higher the reflux ratio, the higher the reboiler duty and the lower the number of stages required to achieve the desired separation. The optimal reflux ratio is observed at the 8th stage at 25725.64kg/hr reboiler duty. The plots of the minimum reflux ratio and total reflux ratio are shown in Figures 6 and 7. It is observed from Figure 6 that the minimum reflux ratio is attained at 1.42 and an equilibrium point, x_f, when there is an infinite number of stages. Figure 8 shows the result of the total reflux ratio when there's a minimum number of stages for the separation, the point where the stripping and enriching lines lie on the 45-degree line when the reflux ratio is 8. The result of the effect of volatility on the number of stages is shown in Table 7. It was also observed that the higher the relative volatility, the fewer the number of stages required to achieve the desired separation while the reboiler duty remains constant.

Simulation of the Extractive Distillation Process

The developed mathematical model for the extractive distillation process was simulated using MATLAB graphical user interface (GUI), as shown in Figure 8, where the input parameters will be supplied, and the result will also be displayed. The result of the simulation of the extractive distillation column and the result of the conventional distillation column are shown in Figure 9.

Extractive Distillation Model Validation

The extractive distillation model developed was validated using ASPEN PLUS v11. Figures 10, 11, and 12 show the validated model's results. Figure 10 shows the process flowsheet for separating ethanol from water using [BMIM] [Br] ionic liquid as an entrainer and Initial Process Design data, Table 8.

Table 6: Effect of Reflux ratio on the number of stages

Reflux ratio	Number of stages	Heat Required(kg/hr)
1.4 (minimum reflux ratio)	39	5612.87
2	14	7016.08
2.5	12	8185.43
3	11	9354.78
3.5	11	10524.13
4	10	11693.47
4.5	10	12862.82
5	10	14032.17
5.5	9	15201.51
6	9	16370.86
7	9	18709.56
8 (total reflux ratio)	8	25725.64

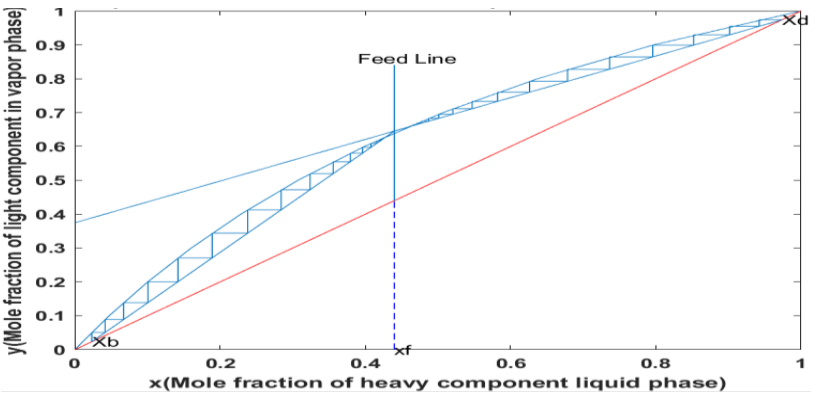


Figure 6: Minimum Reflux Ratio result

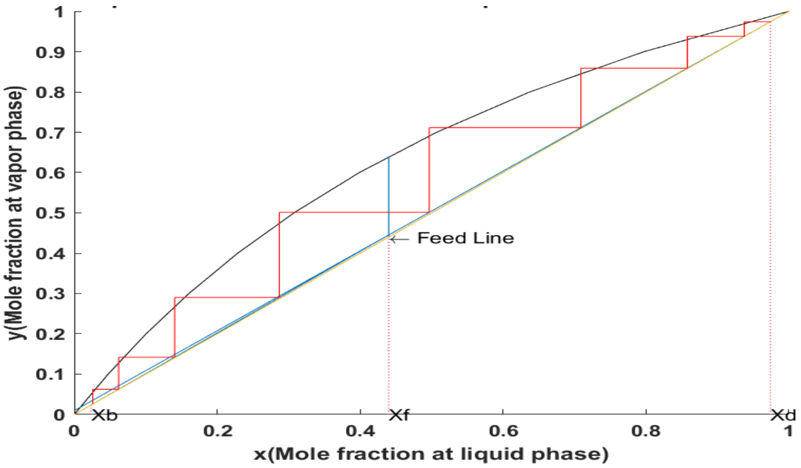
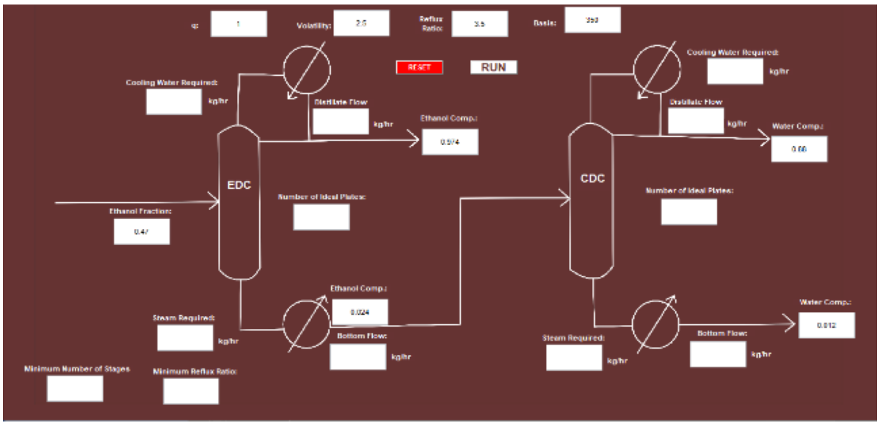


Figure 7: Total reflux ratio result

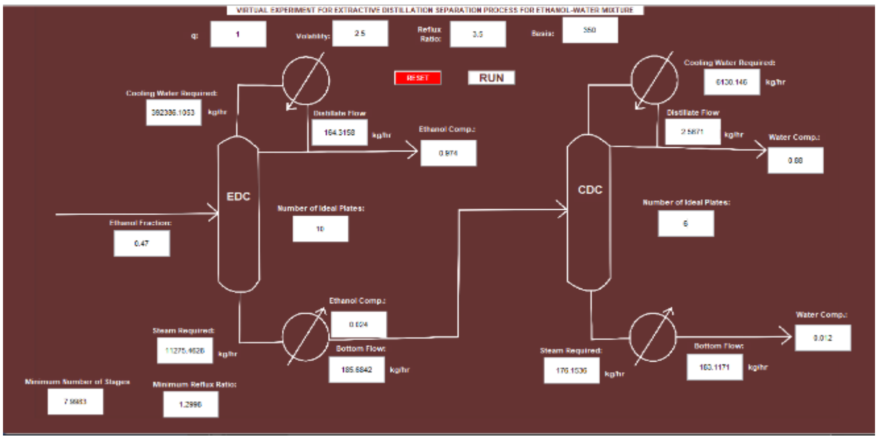
Table 7: Effect of Volatility on number of stages

Volatility	Number of stages	Heat Required(kg/hr)
1.8	24	10524
2	17	10524
2.2	13	10524
2.4	11	10524
2.6	10	10524
2.8	9	10524
3	8	10524
3.2	8	10524
3.4	7	10524
3.6	7	10524
3.8	6	10524
4	6	10524



q: 1
Volatility: 2.5
Reflux Ratio: 3.5
Basis: 350
Ethanol Fraction: 0.47
Ethanol Comp.: 0.974
Ethanol Comp.: 0.024
Water Comp.: 0.88
Water Comp.: 0.012

Figure 8: GUI interface of the extractive distillation model



q: 1
Volatility: 2.5
Reflux Ratio: 3.5
Basis: 350
Cooling Water Required: 382386.1053 kg/hr
Distillate Flow 164.3158 kg/hr
Ethanol Comp.: 0.974
Ethanol Fraction: 0.47
Number of Ideal Plates: 10
Ethanol Comp.: 0.024
Steam Required: 11275.4626 kg/hr
Bottom Flow: 185.6842 kg/hr
Minimum Number of Stages 7.9883
Minimum Reflux Ratio: 1.2996
Cooling Water Required: 6130.146 kg/hr
Distillate Flow 2.5871 kg/hr
Water Comp.: 0.88
Number of Ideal Plates: 6
Water Comp.: 0.012
Steam Required: 176.1536 kg/hr
Bottom Flow: 183.1171 kg/hr

Figure 9: Simulation result for the developed extractive distillation model

Table 8: Initial Process Design data (Hartanto, 2023)

Parameters	Value
Ethanol feed mole-fraction	0.7
Theoretical stage numbers	30
Entrainer mole fraction	0.5
Feed temperature (°C)	25
Entrainer temperature (°C)	70
Binary feed stage	21
Entrainer feed stage	3
Pressure (kPa)	101.3

The flowsheet consists of two main columns: the extractive distillation column (EDC) as the first and the entrainer recovery column (ERC) as the second. The RadFrac block, as a rigorous calculation model, was used to simulate EDC and ERC. The main parameters in EDC that can be used to optimize the separation performance consist of the number of stages (NS), binary feed stage (BFS), entrainer feed stage (EFS), and reflux ratio (RR). The aqueous ethanol solution (FEED stream) and [BMIM] [Br] ionic liquid (SOLVENT stream) enter the EDC. In the first column, ethanol was separated from the water using the entrainer. Higher purity of ethanol (ETHA stream) was obtained in the top column, and a mixture of water/[BMIM] [Br] ionic liquid was achieved in the bottom column. Figure 11 shows the y_x diagram for Ethanol-Water using ASPEN PLUS v11. Figure 11 shows a T-xy diagram for Ethanol-Water using ASPEN PLUS v11. It is observed that the ASPEN simulation model produces results consistent with those obtained using NRTL and WILSON modeled extractive distillation columns in MATLAB, as well as the findings of Chen et al. (2020).

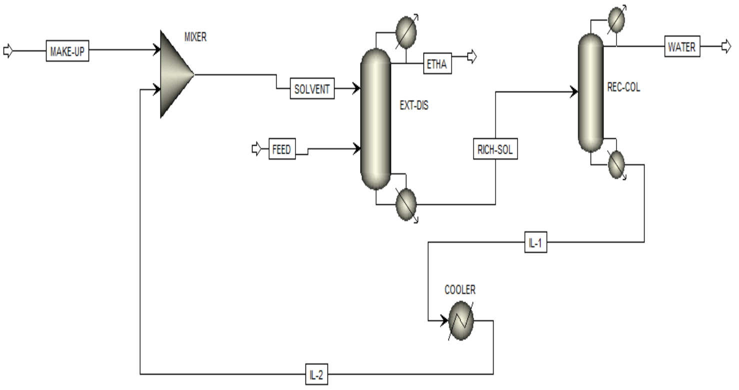


Figure 10: Extractive distillation process flow diagram for ethanol and water with [BMIM] [Br] ionic liquid as an entrainer using ASPEN PLUS v11

The mixture of water/[BMIM] [Br] ionic liquid (RICH-SOL) enters the second column, followed by the separation process. [BMIM] [Br] ionic liquid was collected in the bottom column, and water was obtained in the top column. [BMIM] [Br] ionic liquid (IL-1 stream) was cooled to meet the desired temperature. The cooler [BMIM] [Br] ionic liquid (IL-2) was recycled to the EDC and mixed with the make-up entrainer to keep enough entrainer in the EDC. The result of the simulated flow sheet is shown in Table 9.

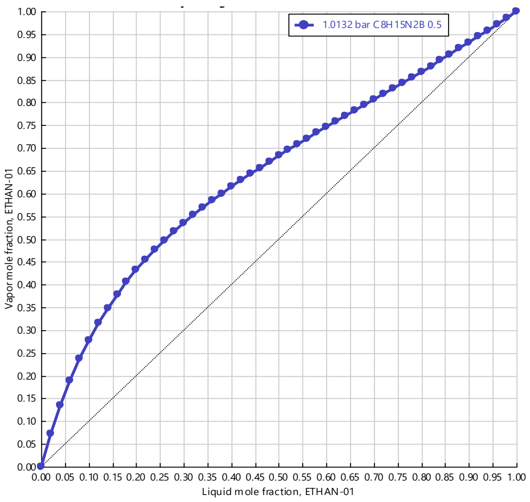


Figure 11: y_x diagram for Ethanol-Water using ASPEN PLUS v11

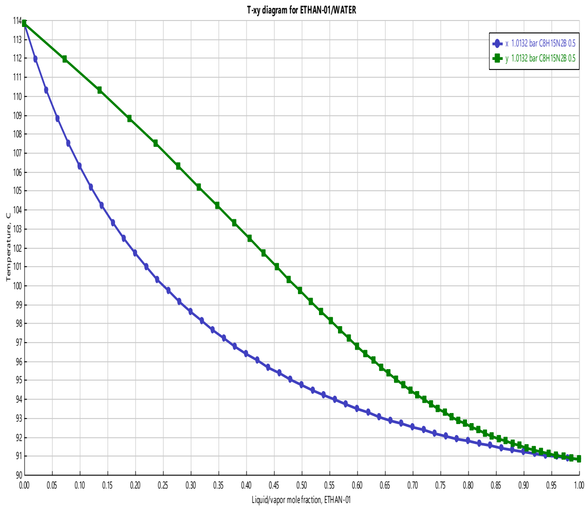


Figure 12: T_xy diagram for ethanol-water using Aspen plus v11

Table 9: Simulation flowsheet of the designed extractive distillation column

Parameters	Extractive Distillation Column	Recovery Distillation Column
Pressure (kPa)	101.3	101.3
Condenser temperature (°C)	78.4	143.5
Condenser heat duty (kW)	-1669.15	-3052.02
Reboiler temperature (°C)	144.2	159.3
Reboiler heat duty (kW)	2513.54	3051.75
Distillate rate (kmol/hr)	60	145
Bottom rate (kmol/h)	145	5
Boil up rate (kmol/h)	174.25	266.28
Molar boils up ratio	1.207	53.255

CONCLUSIONS

Ethanol purification remains a critical challenge in chemical engineering due to the azeotropic nature of ethanol-water mixtures, which limits conventional distillation methods. This study explored extractive distillation as an effective separation technique supported by mathematical modelling and simulation. The McCabe-Thiele and Lewis Sorel methods were used to determine the number of theoretical plates, while Fenske's equation helped estimate the minimum plate requirement. Additionally, Antoine's equation and Raoult's law facilitated accurate vapor-liquid equilibrium (VLE) calculations, with the Non-Random Two-Liquid (NRTL) model proving effective for polar mixtures. It can be concluded that the optimum reflux ratio for the separation is 1.5, the minimum reflux ratio is 1.42, the total reflux ratio is 10, and when the nature of the feed was at saturated liquid, i.e., when q=1, the optimum yield of 99.5% ethanol purity was achieved with minimal reboiler and condenser duty and the number of stages of 8. The implementation of MATLAB R2020a enabled detailed process modelling, simulation and visualization, while validation using ASPEN Plus demonstrated the reliability of the developed model. The findings of this research contribute to the advancement of ethanol purification by providing a comprehensive approach that combines fundamental distillation principles, thermodynamic modelling, and simulation tools. Future studies can focus on experimental validation, optimizing energy consumption, exploring alternative entrainers, and integrating hybrid separation techniques to improve ethanol purification efficiency.

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