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Process Simulation Of Ethylene Glycol-Assisted Extractive Distillation For High-Purity Bioethanol

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Abstract

The practice of ethanol purification has obtained considerable intellectual interest in current discussions owing to its extensive set of applications, including its use as a renewable energy source, an industrial solvent, and in medicinal formulations. Separating ethanol from water is challenging due to the formation of an azeotrope. Extractive distillation is regarded as one of the most advantageous techniques for the separation of ethanol from aqueous solutions, attributable to its favorable energy efficiency and reduced capital expenditure prerequisites. Glycols, particularly ethylene glycol and glycerol, have exhibited considerable effectiveness as solvents in the extractive distillation processes that involve mixtures of ethanol and water. In this study, an extractive distillation simulation of the dehydration of bioethanol process using ethylene glycol as the solvent was conducted. The sensitivity analysis was carried out using the Aspen Plus Simulation to determine the optimal operating conditions. The ***N****on-****R****andom* ***T****wo* ***L****iquid Model (NRTL) thermodynamic model was used in this study. An extensive simulation of the extractive distillation column was ultimately performed, integrating a secondary recovery column for the solvent mixture along with a recycling loop. In the sensitivity analysis, the impact of the number of stages, binary feed stage, entrainer feed stage, reflux ratio (RR) on the purity of ethanol with minimum reboiler and condenser heat duties were studied. The optimal configurations for attaining elevated ethanol concentrations while minimizing energy expenditure in the extractive distillation apparatus consist of 25 stages, a binary feed introduced at stage 22, a solvent feed introduced at stage 3, and a reflux ratio maintained at 1. In the recovery of solvent column, the optimum conditions were found as the number of stages 10, solvent rich feed entry at stage 5 and reflux ratio of 1. Finally, an ethanol purity of 99.7 mole% was achieved with the inclusion of solvent recycling.*

Keywords: *Azeotrope, Ethylene Glycol, Aspen Plus Process Simulator, NRTL, recycling.*

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1. INTRODUCTION

Currently, fossil fuels—including natural gas—remain the dominant sources of energy worldwide. However, these conventional sources are gradually being phased out, primarily due to concerns over carbon dioxide emissions and their environmental impact. In this context, renewable energy options such as solar, wind, and biofuels have emerged as strong alternatives. Among them, bio-ethanol stands out as a particularly promising and impactful renewable energy source because it has the potential to drastically cut greenhouse gas emissions and dependency on fossil fuels (Kumar & Verma, 2024) (Bioethanol, 2022). The ethanol production has increased over the years, mainly considering the growing the world energy demand. A significant proportion of the fuel ethanol generated globally is synthesized through the fermentation of sugars derived from the starches present in various grains, including maize, sorghum, and barley, as well as from the sugars contained in sugarcane and sugar beets (ANP, 2019). Its production from lingocellulosic biomass also offers a sustainable pathway to meet energy demands while addressing environmental concerns. To increase energy generation's efficiency and sustainability as bioethanol production develops, it is essential to investigate cutting-edge technologies and feedstock diversification (Bioethanol, 2022) (Marszałek & Kaminski, 2009).

Achieving high-purity ethanol requires the effective removal of water, typically through distillation. However, the ethanol–water binary system forms a minimum-boiling azeotrope which limits the separation efficiency of conventional distillation methods (Raosaheb, 2015; Guzman-Martinez et al., 2019). To effectively tackle this specific challenge, numerous alternative methodologies have been explored for the separation of ethanol from water, surpassing conventional distillation methods. Solar distillation has been applied as a sustainable approach, but its effectiveness is limited, achieving ethanol concentrations of only up to 80% v/v (Vorayos et al., 2006). Membrane-based separation methodologies, encompassing traditional pervaporation as well as pervaporation synergistically integrated with dynamic control mechanisms, have evidenced their capability to generate anhydrous ethanol (Meireles et al., 2016; Luyben, 2009). Despite their potential, these membrane-based processes suffer from several limitations, such as the complex fabrication of high-performance membranes, reduced separation efficiency due to membrane plasticization, and challenges in scaling up for industrial production. Adsorption-based methods have also been considered for ethanol dehydration (Zheng et al., 2023). However, their application at a commercial scale is hindered by operational complexity and the requirement for intricate adsorber-desorber systems. Among these, extractive and azeotropic distillation are the most widely employed in industrial practice due to their effectiveness in breaking the azeotrope and achieving anhydrous ethanol. The two main methods used in industry for ethanol dehydration are extractive and azeotrope distillation (Kiss and Suszwalak, 2012). Because it uses less energy—up to 30.3% less—extractive distillation outperforms azeotrope distillation (Arifin and Chien, 2008). Consequently, extractive distillation is the recommended method. Ethylene glycol is widely regarded as one of the most prevalent solvents employed in extractive distillation methodologies (Sprakel et al., 2018).

In this study, a process simulation of ethylene glycol-assisted extractive distillation for purification of bioethanol was conducted in Aspen Plus™ V11. The influence of key process parameters—such as the number of stages, feed stage location for the ethanol–water mixture, solvent feed stage, and reflux ratio—was investigated with the objective of maximizing ethanol purity while minimizing reboiler and condenser heat duties. Additionally, a recovery distillation column was incorporated to regenerate and recycle ethylene glycol, enhancing the overall efficiency and sustainability of the process.

2. MATERIALS AND METHODS

2.1 Materials

In this simulation, ethanol, water and ethylene glycol were used from the Aspen Plus data base. The properties are shown in the following table.1.

Table 1: Property table for Ethanol, Water and ethylene glycol

Property	**Ethanol (C_2H_5OH)**	**Water (H_2O)**	**Ethylene Glycol ($C_2H_6O_2$)**
Molecular Formula	C_2H_6O	H_2O	$C_2H_6O_2$
Molecular weight (g/mol)	46.07	18.02	62.07
Boiling Point (°C)	78.4	100.00	197.3
Melting Point (°C)	-114.1	0.00	-12.9

2.2 Methods

Extractive Distillation Simulation

The extractive distillation process for purification of bioethanol was simulated using Aspen Plus™ V11 under steady-state conditions. The NRTL (Non-Random Two-Liquid) model was employed to accurately account for the liquid-phase non-ideality of the ethanol–water–solvent system. Ethylene glycol (EG) was chosen as the entrainer to modify the relative volatilities of the ethanol in aqueous mixtures, thereby facilitating the production of high-purity bioethanol. Figure 1 illustrates the simulation flowsheet, which shows both the extractive distillation unit and the solvent recovery unit, along with a solvent recycling loop to enhance process efficiency and sustainability.

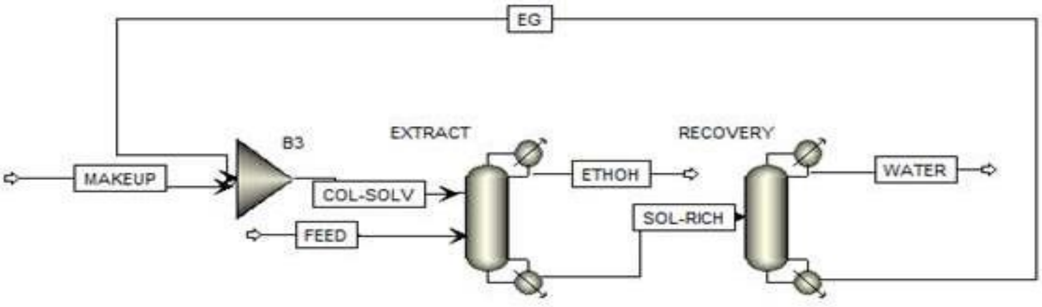

Fig.1. Extractive Distillation simulation flow sheet

The details of the azeotrope formation in the ethanol-water-ethylene glycol ternary mixture were obtained from the Aspen Plus which was shown in table.2. It shows at 78.15

Table 2: Azeotrope formation for Ethanol-water-EG ternary mixture on mole basis

Temperature(°C)	**Classification**	**Type**	**Number of components**	**Ethanol**	**Water**	**Ethylene Glycol**
78.15	Unstable Node	Homogeneous	2	0.8952	0.1048	0.000

The Figure 2 represents the compositional evolution of the liquid residue during distillation. Ethanol, with the lowest boiling point (78.31°C), forms an unstable node**,** indicated by residue curves diverging from its vicinity. Water acts as a saddle point, while ethylene glycol (boiling point 197.25°C) serves as a stable node, attracting most of the residue curves. The map, constructed on a mole basis, demonstrates a homogeneous system and reveals that simple distillation is insufficient for achieving anhydrous ethanol due to the azeotropic behavior. The presence of ethylene glycol effectively alters the residue path, enabling the system to bypass the azeotrope and favor ethanol dehydration. This supports the use of extractive distillation with ethylene glycol as a suitable entrainer for industrial ethanol purification.

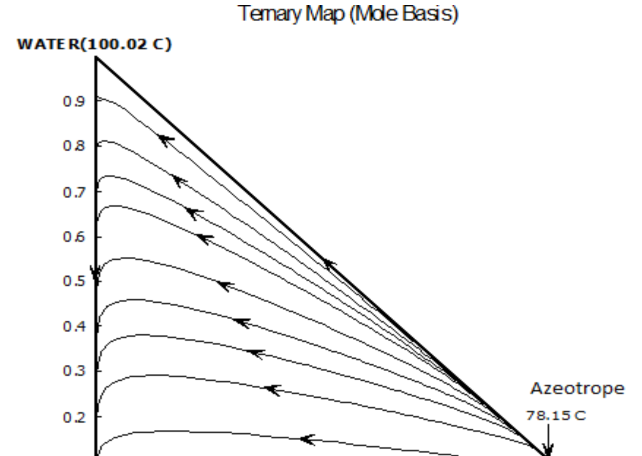

Figure 2: Residue curves for the ternary mixture

Table 3: Operating conditions of the extractive distillation unit

Parameter	**Value**
Feed Flow rate (kmol/hr)	100
Feed Temperature (°C)	78
Ethanol feed mole fraction	0.87
Distillate molar flow (kmol/hr)	87
Number of stages	50
Binary Feed Stage	10
Entrainer molar rate (kmol/hr)	50
Entrainer Feed Stage	5
Reflux ratio (RR)	0.5
Entrainer temperature (°C)	25
Pressure (atm)	1

In table 3 illustrates the initial operating conditions in Aspen Plus Simulator. A significant proportion of scholarly articles pertaining to extractive and azeotropic distillation methodologies in the existing literature typically employ a stage range of 20 to 50. Hence 50 stages were selected in the column. Binary feed stage and entrainer stages were selected as 10 and 5 respectively, whereas reflux ratio was chosen to be 0.5. The entrainer to feed ratio (S/F) was 0.5.

A thorough sensitivity analysis was performed to clarify the influence of multiple parameters, such as the quantity of stages, binary feed stages, entrainer feed stages, and the reflux ratio, on both the purity of ethanol and the energy demands of the condenser and reboiler systems.

Recovery Column for Ethylene Glycol

Based on the findings derived from the sensitivity analysis, optimal parameters for the binary feed tray, entrainer stage, reflux ratio, reboiler and condenser duties, as well as the number of stages within the extractive distillation column, a recovery distillation column dedicated to ethylene glycol was integrated with the bottom stream of the initial column, which was enriched with the introduced entrainer. There were ten number of stages in the recovery column with reflux ratio of 1. The bottom molar flow rate was given based material availability and further sensitivity analysis was performed for optimum parameters for the maximum of ethylene glycol recovery.

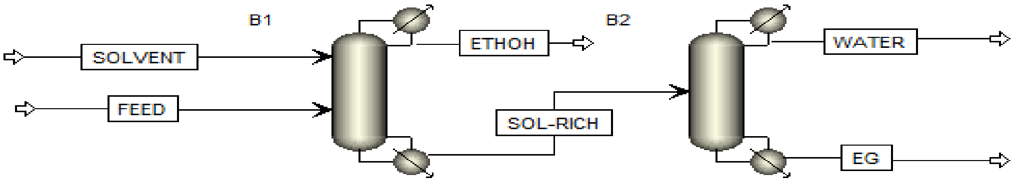

Figure 4: Extractive and Recovery distillation columns

The effluent obtained from the lower area of the recovery column was fed back into the extractive distillation column to secure the highest level of efficiency in solvent expenditure. The overall optimal conditions were determined through sensitivity analysis.

3. RESULTS AND DISCUSSIONS

3.1 Sensitivity analysis Study

A thorough sensitivity analysis was carried out to examine the influence of multiple parameters, encompassing the quantity of stages, binary feed stages, entrainer feed stages, and reflux ratio, on the purity of ethanol and the energy demands of the condenser and reboiler systems. With the initial operating conditions in the first column, we were able to get only 98.5 mol% purity of ethanol in the distillate. The results of the streams were shown in the table 4.

Table 4: Simulation results before the sensitivity analysis

Stream Name	Feed	Solvent	ETHOH (Distillate)	RICH-SOL (Bottoms)
Temperature (°C)	78	25	78.26727496	133.8378028
Feed Flow rate (kmol/hr)	100	50	87	63
Feed ethanol flow rate (kmol/hr)	87	0	85.70291177	1.297088231
Feed water flow rate (kmol/hr)	13	0	1.296477885	11.70352211
Entrainer flow rate (kmol/hr)	0	50	0.000610346	49.99938965
Molar fraction of Ethanol	0.87	0	0.98509094	0.020588702
Molar fraction of water	0.13	0	0.014902045	0.185770192
Molar fraction of entrainer	0	1	7.01547E-06	0.793641106

The influence of the variation in the number of stages and the molar reflux ratio (RR) on the purity of ethanol in the overhead product is depicted in the figure 5; it illustrates that as the number of stages is increased, the purity of ethanol increases and subsequently stabilizes, remaining nearly constant from stages 25 to 50. The reflux ratio of 1.0, demonstrated superior purity in comparison to the alternative reflux ratios. This indicates that the process of extractive distillation can be effectively conducted at 25 stages and a reflux ratio of 1, which serves as the optimal condition.

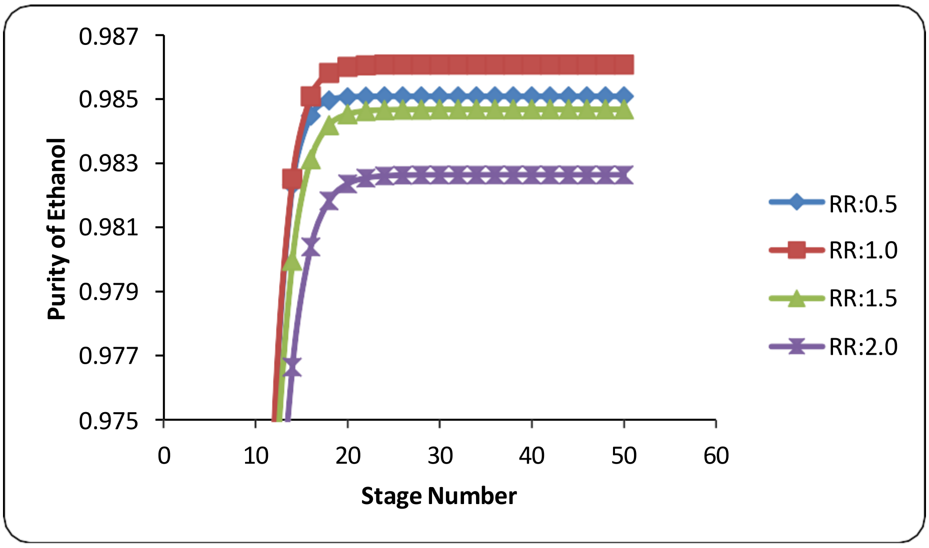

Figure 5: The impact of the no. of stages and RR to the purity of ethanol

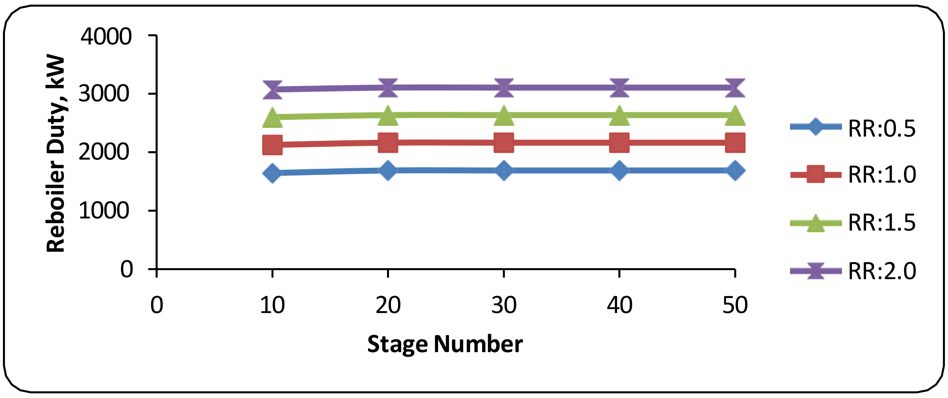

Figure 6: The impact of the number of stages and RR to the reboiler duty

The impact of the number of stages and the reflux ratio on the heat duties of the reboiler and condenser was systematically examined as illustrated in Figures 6 and 7, respectively. The total number of stages did not demonstrate a notable effect on the duties in both cases; however, the reflux ratio indicated a substantial impact. An increase in the reflux ratio corresponded with a rise in the duties for both components. The duties attained their peak at a reflux ratio of 2. Nevertheless, since a reflux ratio of 1 was identified as optimal from Figure 5, this same reflux ratio of 1 was subsequently regarded as the most favorable condition.

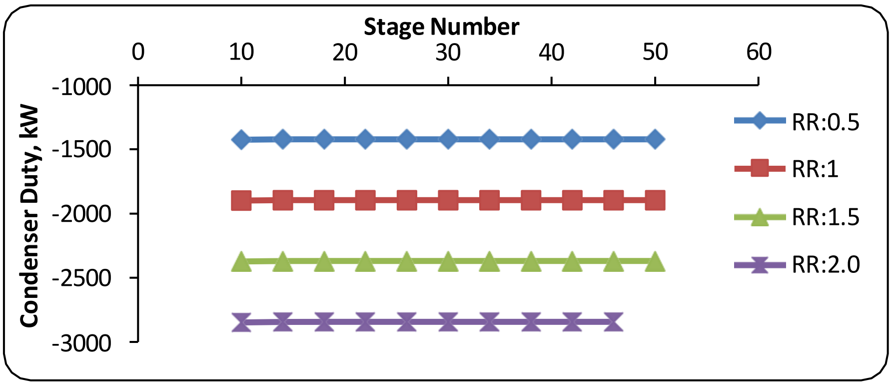

Figure 7: The impact of the number of stages and RR to the condenser duty

Figure 8 illustrates how the reflux ratio and binary feed stage affect the distillate's ethanol purity. With a reflux ratio of 1, the binary feed stage produces the greatest results in stages 20 to 40. Since 25 were determined to be the optimal number of stages in the extractive distillation column, the binary feed stage at 22 was considered to be optimal value.

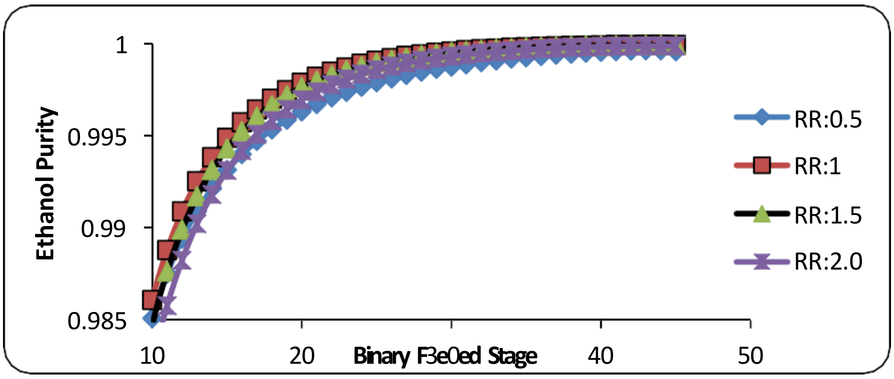

Figure 8: The impact of binary feed stage and RR to the ethanol purity

Figure 9 illustrates the impact of the entrainer stage and reflux ratio to the distillate's ethanol purity. The entrainer stage 2 to 3 give the best purity of ethanol in the distillate for the given input conditions.

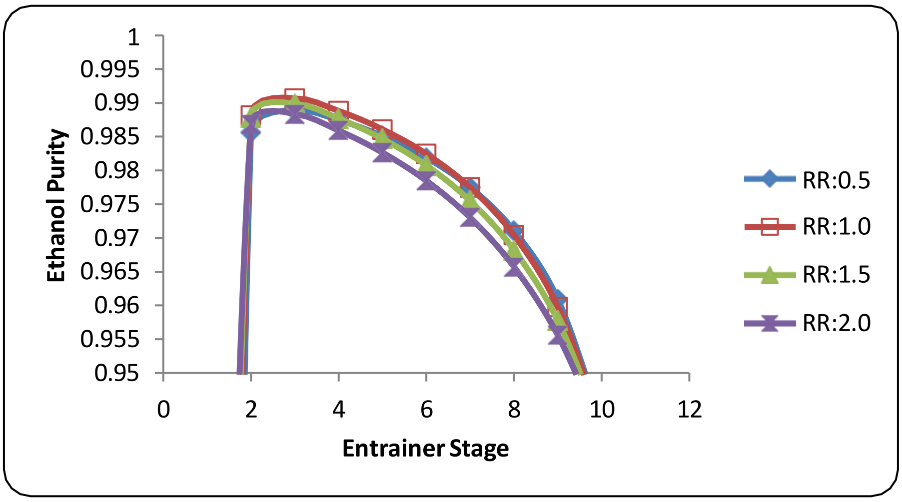

Figure 9: The impact of the entrainer stage and RR to the ethanol purity

3.2. Simulation Results

Based on the sensitivity results, the optimal parameters were used for the extractive and recovery columns design. The optimal design parameters for the both columns were shown in the table 5. The simulation results with the recycling of the ethylene glycol (EG) stream showed 99.5 mole% purity of ethanol in the distillate.

Table 5: Extractive and Recovery column optimum design parameters

Parameter	Extractive Distillation Column	Recovery Distillation Column
Feed Flow rate (kmol/hr)	100	-
Feed Temperature (°C)	78	143.148
Ethanol feed mole fraction	0.87	-
Total Number of Stages	25	10
Distillate molar flow (kmol/hr)	87	-
Bottoms molar rate (kmol/hr)	-	50
Binary Feed Stage	22	3
Entrainer molar rate (kmol/hr)	50	-
Entrainer Feed Stage	3	-
Reflux ratio (RR)	1	1

Table 6 illustrates the final results of the simulation with recycling of the entrainer. To achieve a high purity of bioethanol in the distillate (ETHOH), which was about 99.7 mole% pure ethanol, extractive distillation was carried out using a binary feed of 100 kmol/hr and a makeup solvent (MAKEUP) of 0.075 kmol/hr. The majority of the ethylene glycol and water was identified in the bottoms (SOL-RICH) of the extractive distillation, which yielded a total of 63.075 kmol/hr. Pure entrainer was recovered from the bottoms of the second column using distillation. The bottoms (EG) of the recovery column, which contained 99.9 mol% ethylene glycol. At almost 97.5%, water was gathered as the second column's top product. To make the best use of it, the EG stream was recycled to the first column.

Table 6: Results of the extraction distillation

Stream Name	**Feed**	**ETHOH**	**SOL-RICH**	**COL-SOLV**	**MAKEUP**	**EG**	**WATER**
Temperature (°C)	78	78.307	143.148	196.358	25	196.58	94.768
Mole Flows (kmol/hr)	100	87	63.075	50.075	0.075	50	13.075
Ethanol (kmol/hr)	87	86.724	0.277	0.001	0	0.001	0.277
Water (kmol/hr)	13	0.257	12.818	0.075	0	0.075	12.744
Ethylene Glycol(kmol/hr)	0	0.02	49.981	50	0.075	49.926	0.055
Mole fraction of Ethanol	0.87	**0.997**	0.005	0.001	0	0.001	0.022
Mole fraction of Water	0.13	0.003	0.204	0.002	0	0.002	**0.975**
Mole fraction of Ethylene Glycol	0	0.001	0.793	0.999	1	**0.999**	0.005

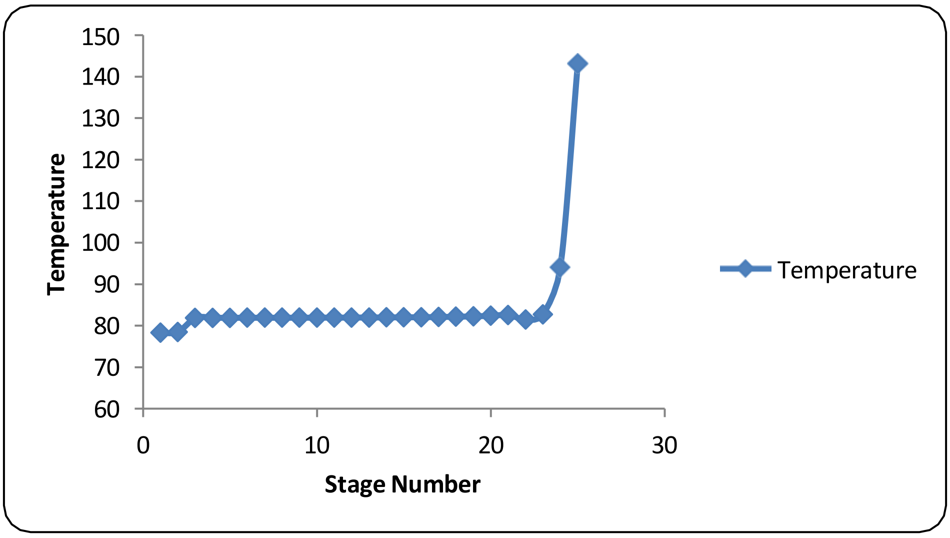

Figure 10: Temperature profile over the stages

Figure 10 displayed the temperature change over the stages. It indicates that the temperature is lowest at the top of the distillation (78.3 °C) and highest at the bottoms (143.148 °C). Ethanol, water, and ethylene glycol compositions were compared throughout the steps in Figure 11. Since the feed was added at step 22, the water composition increased from stage 20. The entrainer was shifted to the bottom of the column because it was a less volatile component, while the maximum amount of ethanol vapor was attained at the top.

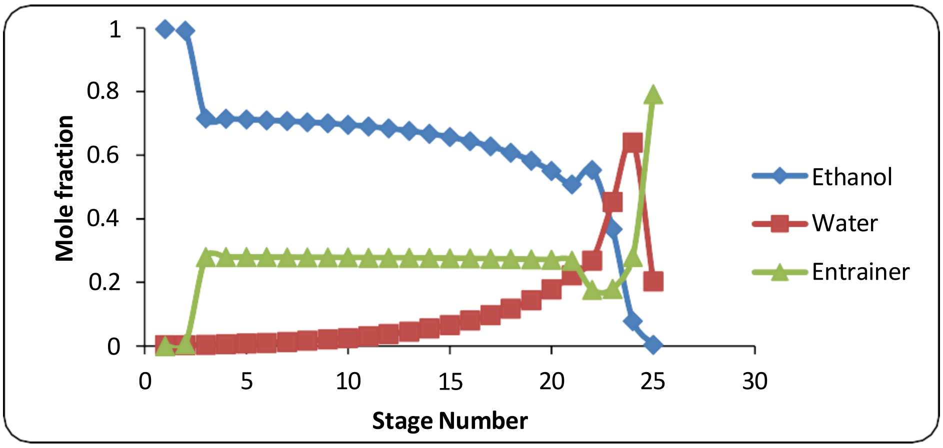

Figure 11: Liquid composition profiles over the stages

4. CONCLUSIONS

The Process simulation for high purity bio-ethanol using extractive distillation was successfully performed in Aspen Plus simulator. The NRTL thermodynamic model was applied for property estimation. The solvent, ethylene glycol as an entrainer was proved to be an effective in producing high purity ethanol. The sensitivity analysis was performed for the both extractive and recovery columns and optimal configuration for the design of columns was obtained as 25 number of stages, reflux ratio of 1, binary feed stages as 22 and entriner feed stage as 3. The high purity bioethanol of 99.7 mole % was achieved and 99.9 mole% purity ethylene glycol was recovered and recycled to the extractive column.

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