Simulation of the Extractive Distillation using Ethylene Glycol as an Entrainer in the Bioethanol Dehydration

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Abstract: In this work, the dehydration of bioethanol via extractive distillation using ethylene glycol as an entrainer was simulated using Aspen Plus software platform. RadFrac module for distillation was performed including column for the ethylene glycol recovery which represented the industrial condition. The Non Random Two Liquids-Hayden-O'Connell (NRTL-HOC) thermodynamic model was used in the simulation. The results show that the possibility of producing high purity bioethanol through the extractive distillation using ethylene glycol as an entrainer. The most suitable configuration in extractive distillation column is 23 theoritical stages with the best binary and entrainer feeding stages are 13 and 23, respectively using ethylene glycol as an entrainer with reflux ratio of 2. The effect of main variables to the extractive distillation were also obtained.

1 INTRODUCTION

The use of alternatif energy become an important concern for human kind to reduce the draw back of the conventional fuel. Biofuels such as bioethanol and biodiesel have been significantly performed as subtitutes for fossil fuel energy such as gasoline and diesel fuel especially in the transportation sector. Bioethanol is known as a worldwide interest for the renewable energy because its high energy content and can be produced from the renewable sources mainly through the fermentation of sugar . The production of bioethanol through fermentation process yielding the purity of 7-12 wt% (Zabed et al., 2017). Conventional distillation used in the purification of bioethanol can only produced the maximum purity of 95.6 wt% due to azeotrope form of ethanol and water (Dias et al., 2009). On the other hand, ethanol as a fuel purposes should have the minimum purifty of 99.5 wt% to meet the product specification (Zhu et al., 2016).

Several methods were employed to produce high grade bioethanol such as azeotropic distillation, adsorption using molecular sieve, pervoration membranes, and extractive distillation (Xu et al., 2018) (Frolkova and Raeva, 2010) (Seo et al., 2018) (Kiss and Suszwalak, 2012). Extractive distillation has been widely used in the industry as a proven technology because it has low energy consumption (Fu, 2004). Feasible entrainer was used in the extractive distillation to break the azeotrope (Hartanto et al., 2016). Ethlyne glycol is possible entrainer proposed to break the azeotrope of ethanol-water (Kamihama et al., 2012).

Isobaric vapor-liquid equilibria is the basic data which can be used to optimize the column design (Hardjono et al., 2017). The vapor-liquid equilibria can be obtained from experimental and prediction (Hartanto, Mustain and Nugroho, 2017). In the

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extractive distillation, several research were conducted to calculate or simulated the extractive distillation of ethanol dehydration using ethylene glycol as an entrainer. Black and Ditsler was reported the comparison of the calculation between the use of ehtylne glycol and n-pentane in extractive distillation (Black and Ditsler, 1972). Anisuzzaman et al. also simulated the extractive distillation using three solvents of 1,3-butylene glycol, mixture 1,3-butylene glycol and ethylene glycol, and mixture 1,3-butylene glycol and glycol ethyl ether using the Aspen HYSYS Platform (Anisuzzaman et al., 2018). The mixture of ethylene glycol – calcium chloride was used in the extractive distillation of ethanol dehydration simulation using the Aspen Plus platform (Gil et al., 2008). The experimental and pilot scale research of extractive distillation using ethlyne glycol as a solvent were conducted by Meirelles(Yeh and Berg, 1992). Gil et al. used glycol-glycerol as an entrainer in the simulation of ethanol dehydration using Aspen Plus software platform (Gil, García and Rodríguez, 2014).

The study of the extractive distillation for the bioethanol dehydration using ethylene glycol as an entrainer using the Aspen Plus software platform is not available in the published literature. In this study, the effect of stages, reflux ratio (RR), entrainer stage, binary feed stage to product composition, reboiler and condensor duty, and energy duty were investigated. The NRTL-HOC model was used as a thermodynamic package in the simulation.

2 EXTRACTIVE DISTILLATION SIMULATION

The extractive distilation simulation was presented in Figure 1 as a process flow diagram which consist of two columns, one as a extractive distillation column and one as an entrainer recovery column.

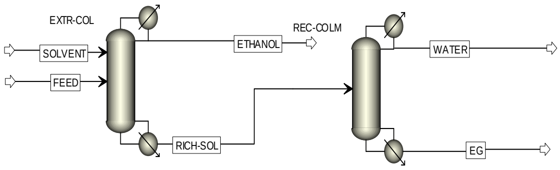

Figure 1: Process flow diagram for the extractive distillation using ethylene glycol as an entrainer.

The isobaric vapor liquid equilibria of ethanol-water-ethylene glycol was taken from the reference (Kamihama et al., 2012). The simulation was conducted using The NRTL-HOC model as a thermodynamic package. The binary interaction parameter of ethanol-water, ethanol-ethylne glycol, and water--ethylne glycol was taken from Aspen database which shown in Table 1 with the unit of *K*.

Table 1: Binary Interaction Parameters*.

Component	Parameters		
	Aij	***Aji***	***Cij***
ethanol-water	227.56	5196.9	0.4
ethanol-ethylne glycol	1035.6	708.38	0.23
water--ethylne	-2510	2731.3	0.33

*Taken from Aspen Plus physical property databank

The extended Antoine was used in this simulation to calculate the total pressure and vapor pressure of the component. The Antoine parameters was listed in the Table 2 with the unit pressure and temperature are *kPa* and *K*, respectively.

Table 2: Extended Antoine Parameters*.

Parameters	**Compound**		
	ethanol	water	ethylene glycol
A_1	74.1675	58.2467	-418.74
A_2	-7827.8	6842.91	7736.16
A_3	0	0	0
A_4	-0.00185	0.00278	-0.0872
A_5	-7.96131	-6.13638	72.7647
$10^{-15} A_6$	0.023	0.0033	0.017
A_7	6	6	6
A_8	302.559	319.267	406.541
A_9	516.2	647.3	645

*Taken from Aspen Plus physical property databank

Some of physical properties were used in the calculation of phase equilibrium such as critical temperature (*Tc*), critical pressure (*Pc*), critical volume (*Vc*), compressibility factor (*Zc*), dipole moment (μ), and acentric factor (ω) of each component. The constant of each physical property listed in Table 3.

Table 3: Physical Properties Of Pure Component*.

Parameters	**Compound**		
	ethanol	water	ethylene glycol
Tc (K)	516.2	647.3	645
Pc (kPa)	6383.48	22048.3	7700.7
Vc (m^3/kmol)	0.16673	0.05589	0.18802
Zc	0.248	0.229	0.27
μ *(debye)*	1.7	1.8	2.2
ω	0.635	0.344	1.17921

*Taken from Aspen Plus physical property databank

The simulation were conducted with 50 theoritical stages in the extractive distillation column. The mol fraction of entrainer used for all simulation is fixed at 0.059 according to the optimum amount of entrainer which added into the system to break the azeotrope of ethanol-water (Kamihama et al., 2012). The initial input data of the simulation are listed in the Table 4.

Table 4: Process Design Parameters.

Parameters	Value
Feed flowrate (kmol/h)	94.1
Distillate mole flow (kmol/h)	75.28
Ethanol feed mole fraction	0.8
Theoritical stage numbers	50
Entrainer mole fraction	0.059
Feed temperature (^oC)	25
Entrainer temperature (^oC)	25
Binary feed stage	10
Entrainer feed stage	5
Pressure (*kPa*)	101.3

3 RESULTS AND DISCUSSION

3.1 Sensivity Analysis Results

In this work number of stages, reflux ratio, feed stage, entrainer feed stage, binary feed stage, and entrainer mole flow were analyzed. The effect of the number of stage and reflux ratio to the compositions of ethanol in the distillate (x_D) reported in Figure 2. The higher reflux ratio give the higher purity of the ethanol in the distillate because more contact between liquid and vapor occured in the extractive distillation column. The highest x_D can be obtained from the reflux ratio of 2. The ethanol concentration changed significantly from stage 1 until stage 20 and remains constant at number of stage range from 20 to 50. It show that the extractive distillation column can be operated in 20 stages and at a reflux ratio of 2 as an optimal condition.

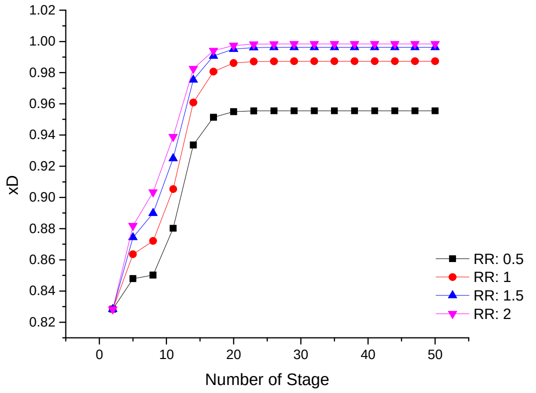

Figure 2: The effect of the number of stages and reflux ratio to the ethanol composition in the distillate.

The effect of the number of stages and reflux ratio to the reboiler and condensor duty were analyzed in Figure 3 and Figure 4, respectively. The number of stages did not change the duties for both cases, but the relux ratio give the significant effect. It means that the extractive distillation column energy consumption was influenced by the relux ratio. From these results, it can be concluded that the optimal reflux ratio is 2 which can save the energy consumption.

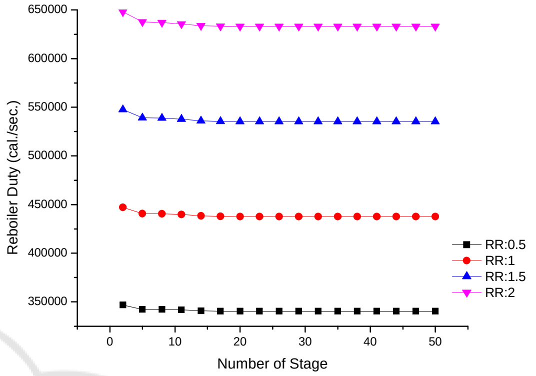

Figure 3: The effect of the number of stages and reflux ratio to the reboiler duty.

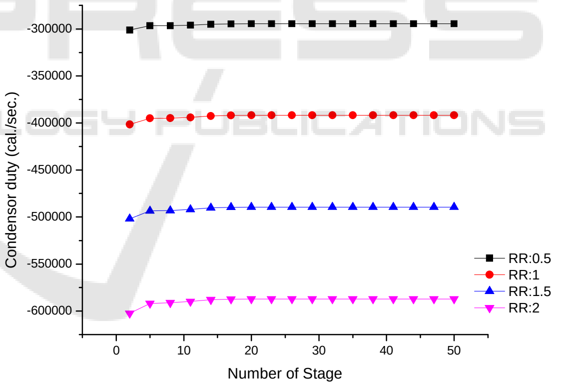

Figure 4: The effect of the number of stages and reflux ratio to the condensor duty.

The effect of binary feed stage and reflux ratio to the ethanol composition in the distillate is shown in Figure 5. The binary feed stage give the best result in stages 13 to 40 with the reflux ratio of 2. These stages give longer and optimal contact between feed and entrainer. The decreasing of the ethanol composition occured in stages 40 to 50 because in this stages, feed position is near the bottom and reboiler thus it have high possibility become vapor phase.

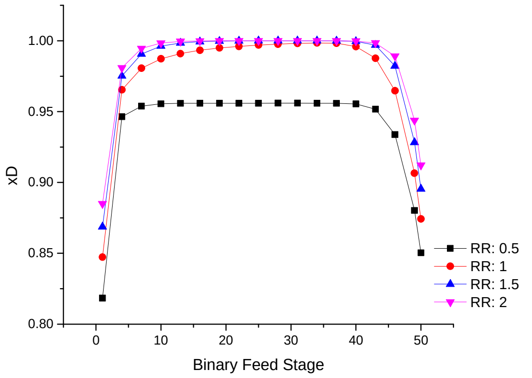

Figure 5: The effect of the binary feed stage and reflux ratio the ethanol composition in the distillate.

Figure 6 shows the entrainer feed stage reach the optimal results at stage 3. It is reported that the highest ethanol composition in the distillate were obtained at reflux ratio of 2. The ethanol composition was constant at entrainer feed stages from 3-50 because the best interaction between feed and entrainer occured in a liquid phase. The entrainer predominantly in liquid phase when fed in the top and all stages below the top. Entrainer tend to vapor phase when it fed in the bottom.

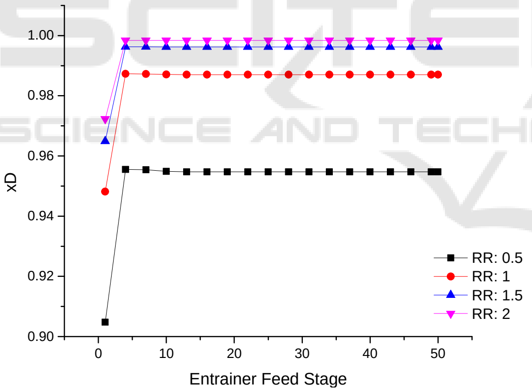

Figure 6: The effect of the entrainer stage and reflux ratio the ethanol composition in the distillate.

3.2 Simulation Results

Two columns are involved in the extractive distillation simulation to separate ethanol from water using ethylene glycol as an entrainer. The first column was the extractive distillation column which produced ethanol with purity of 99.8% (mole fraction). The second column was ethylene glycol recovery column which the purity of ethylene glycol can be recovered was 99.6% (mole fraction). The comparison the effect of the number of stages to the mole fraction of ethanol, water, and ethylene glycol was shown in Figure 7. The optimum configuration and operating conditions obtained in the simulation for the extractive distillation and recovery column are shown in Tables 5 and 6.

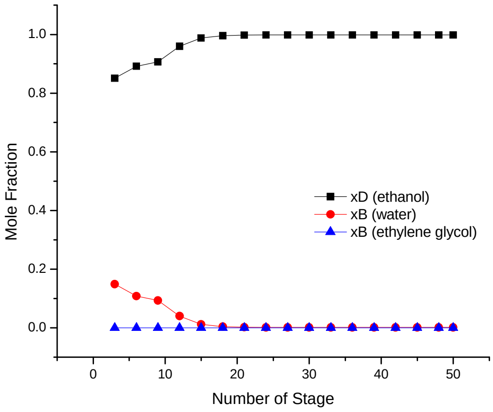

Figure 7: The effect of the number of stages to ethanol composition in the distillate, and water and ethylene glycol compositions in the bottom.

Table 5: Extractive Distillation Column Design.

Parameters	**Value**
Number of stage	23
Binary feed stage	13
Entrainer feed stage	5
Reflux ratio	2
Entrainer molar ratio	0.059
Entrainer temperature (°C)	25
Distillate mole flow (kmol/h)	78.28

Table 6: Recovery Column Design.

Parameters	**Value**
Number of stage	17
Distillate mole flow (kmol/h)	18.8
Feed stage	12
Reflux ratio	1
Bottom temperature (°C)	469.48
Distillate temperature (°C)	99.25
Distillate mole flow (kmol/h)	18.8

4 CONCLUSIONS

The simulation show the optimal operating condition to separate the azeotropic mixture of ethanol and water using ethylene glycol as an entrainer. The sensivity analysis were conducted to obtain the best condition and configuration for the extractive distillation column and recovery column. The composition of high purity of ethanol and energy required were consistent. Ethylene glycol is one of the suitable entrainer which can be used to separate the azeotrope in ethanol-water mixture to obtain high grade bioethanol.

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