Design and Optimization of Isopropyl Alcohol-Water Separation using Heterogenous Azeotropic Distillation

Emelia Kezia Lasut [a,1], Yansen Hartanto [a,2,*], Herry Santoso [a,3]

[a] Department of Chemical Engineering, Faculty of Industrial Technology, Universitas Katolik Parahyangan, Jln. Ciumbuleuit No. 92, Bandung, 40141
[1] 6216104@student.unpar.ac.id; [2] yansen_hartanto@unpar.ac.id*; [3] herry72@yahoo.com
* corresponding author

ARTICLE INFO

Article history
Received September 06, 2021
Revised January 07, 2022
Accepted January 18, 2022

Keywords
Azeotropic
Distillation
Entrainer
Heterogenous
Optimization

ABSTRACT

Heterogeneous azeotropic distillation is one technique of separating the mixtures that form azeotropes. In this research, a case study will be carried out on separating a mixture of isopropyl alcohol (IPA) and water where this mixture forms an azeotropic point. IPA is an alcohol that can be converted into diesel fuel through an esterification reaction. This study will use the Aspen Plus v8.8 simulator. The entrainer used were benzene and cyclohexane. The thermodynamic model used was NRTL. The configuration used in this study consists of two distillation columns with one decanter to separate the ternary azeotropic points. Optimization is carried out sequentially by changing one variable while the other variables are kept constant. The variables used are the number of stages, and the location of the feed entered in each column. The objective function used in this optimization is the Total Annual Cost (TAC). This research obtained a heterogeneous azeotropic distillation configuration that produced high-purity IPA and water products. Based on the optimization results, the benzene entrainer is cheaper than the cyclohexane entrainer.

1. Introduction

The demand for energy sources and the increasingly negative impact caused by fossil fuels has prompted studies on the use of alternative fuels such as bio-based fuels. One alternative is alcohol as a fuel, such as isopropyl alcohol (IPA), which has been produced from petroleum products. IPA can be made from biomass materials through biomass fermentation [1]. This material can be converted into biodiesel through an esterification reaction [2]. However, separating isopropyl alcohol from water is quite tricky due to the azeotrope point produced by the two mixtures at a temperature of 80.3 ºC and composition of 68.1%-mole IPA [3].

The azeotrope point occurs when the liquid and vapor composition are equal due to a mixture's non-ideal nature [4]. The existence of an azeotrope point causes the mixture cannot be separated by ordinary distillation because the purity of one of the products is at that azeotropic point [5]. Special techniques such as a membrane or azeotropic distillation are needed [6]. Several types of azeotropic distillation can be used, such as pressure swing distillation, extractive distillation, and heterogeneous azeotropic distillation. In the pressure swing distillation, 2 (two) distillation columns are used, which operate at high pressure and low pressure where the azeotrope point will shift due to this pressure change. Meanwhile, in extractive distillation and heterogeneous azeotropic distillation, another component (entrainer) is added to separate the initial azeotropic mixture. In extractive distillation, the entrainer will dissolve one of the components without forming a new azeotropic point. In contrast, in heterogeneous azeotropic distillation, the entrainer will produce a tertiary azeotrope, a liquid-liquid heterogeneous mixture then separated by a decanter [7].

In a previous study by Chien et al. [8], was conducted on the configuration of azeotropic distillation, namely the 2 (two) column configuration, and the 3 (three) column configuration with a cyclohexane entrainer. This research turns out that the configuration of 2 (two) columns results in lower total costs. In a study by Arifin et al. [3], an additional pre concentrator column was used due to the very low alcohol concentration.

This study will examine the effect of the type of entrainer, namely cyclohexane and benzene, on the total cost of separation expressed by the Total Annual Cost (TAC), which considers operating costs and equipment costs.

2. Methodology

2.1. Equipment

This research was conducted using Aspen Plus® software/simulator version 8.8 from Aspentech. The distillation column used was RADFRAC, and the thermodynamic model used was NRTL. RADFRAC is an exact (rigorous) distillation column model on a simulator that uses mass balance, energy balance, and equilibrium calculations at each stage. In comparison, the NRTL thermodynamic model is a good model to represent a not ideal mixture [9].

2.2. Procedure

This research generally consists of 2 (two) stages, namely preliminary design and optimization. The feed used consists of an equimolar mixture of IPA and water. The preliminary design will use design data from the research of Arifin et al. [3] to obtain the initial configuration of heterogeneous azeotropic distillation. The feed used is an IPA-water equimolar mixture on the basis of 100 kmol/hour. The first distillation column is targeted to produce high purity IPA, while the second column produces water. At the optimization stage, it is carried out sequentially by changing the design variables gradually, namely the number of stages of the first distillation column (N_1), the location of the feed in the first distillation column (N_{F1}), the number of stages of the second distillation column (N_2), and the area of the feed in the distillation column. Second (N_{F2}). The minimized objective function is Total Annual Cost (TAC) [10]. The process flow diagram is presented in Figure 1, and the optimization procedure is shown in Figure 2. From Figure 1, it can be seen that the separator configuration consists of 2 distillation columns. In the first distillation column, the feed will contact the entrainer stream coming from the decanter (organic phase). The bottom product of the first column is IPA, while the top product is a tertiary azeotrope which is then separated in the decanter after condensation. The aqueous phase of the decanter will be separated in the second column, which produces water as a bottom product. The top product of the second column will be recycled to the first distillation column.

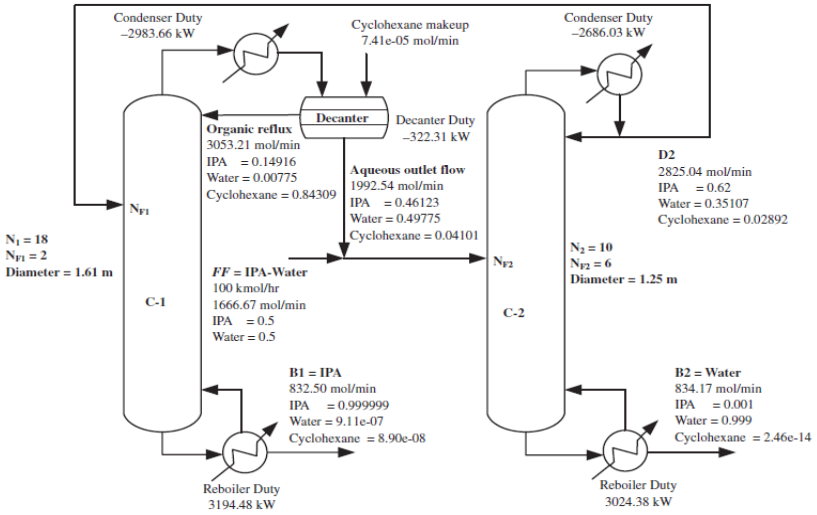

Fig. 1. Process Flow Diagram

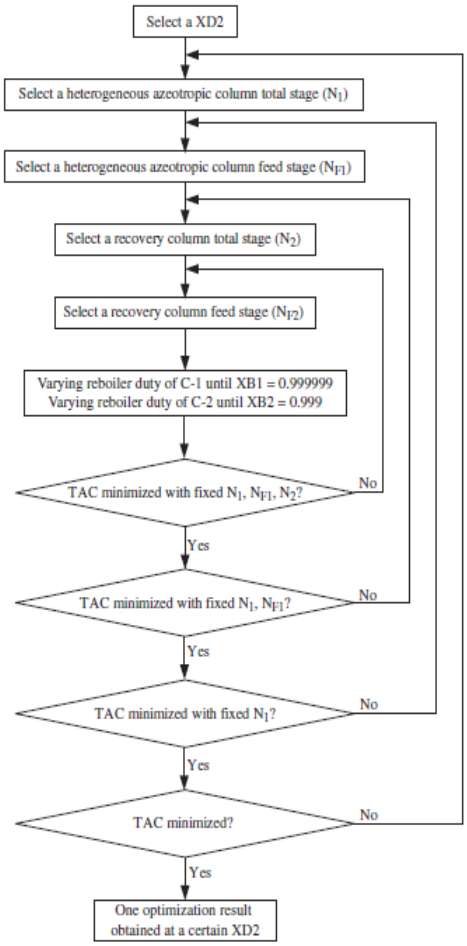

Fig. 2. Sequential Optimization Procedure

3. Results and Discussion

3.1. Preliminary Design and Validation

This study begins with the preliminary design of heterogeneous azeotropic distillation. The aim is to find out whether the initial model made in this study is valid or not. A validity test was carried out by comparing the purity of the IPA and water products and the required condenser and reboiler duty. The process flow diagram for Aspen Plus® is presented in Figure 3.

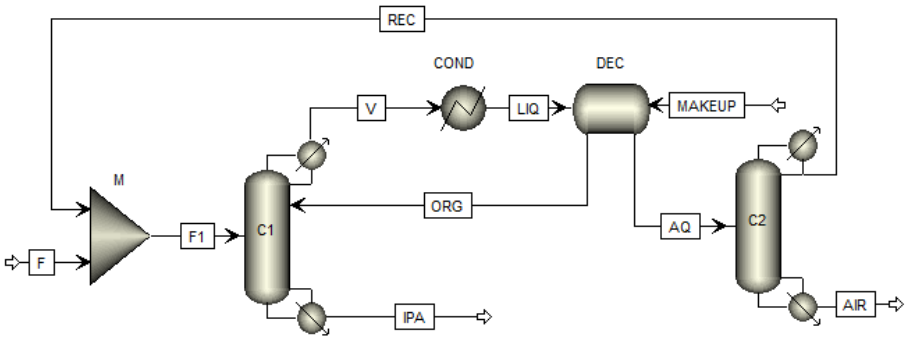

Fig. 3. Process Flow Diagram in Aspen Plus®

The feed is an equimolar isopropyl alcohol (IPA) mixture with water at room temperature and pressure conditions. Both distillation columns operate at atmospheric pressure. The purity of the bottom product is regulated by changing the reboiler duty. In this study, the purity of isopropyl alcohol (mole fraction) is expected to reach 0.99999 and water purity to reach 0.999. The first

distillation column was modeled with a stripper so that the condenser was added to a separate unit. A comparison of the results of this study with literature data [3] is presented in Table 1 and Table 2.

Table 1. Comparison of Distillation Column 1

Variable	Literature [3]	This Study
Reboiler Duty (kW)	3194.48	3393.46
Condenser Duty (kW)	-2923.66	-2989.01
Purity of IPA (mole fraction)	0.99999	0.99999

Table 2. Comparison of Distillation Column 2

Variable	Literature [3]	This Study
Reboiler Duty (kW)	3024.38	3172.86
Condenser Duty (kW)	-2686.03	-2915.63
Purity of Water (mole fraction)	0.999	0.999

From Table 1 and Table 2, the purity of isopropyl alcohol (IPA) and water obtained is the same. Different versions of the simulator were used to cause the difference in condenser and reboiler duty.

3.2. Optimization

The research was continued by performing sequential optimization, namely by changing the number of steps in the first column (N_1), the location of the feed in the first column (N_{F1}), the number of stages in the second column (N_2), and the location of the feed in the second column (N_{F2}). The other variables are kept constant for the same purity for each optimized variable. The objective function used is Total Annual Cost (TAC). The calculation of TAC here is based on the procedure described by Luyben W. L [11]. The optimization procedure will be repeated until the same minimum TAC is obtained to ensure that the optimum point achieved is the optimum global point. The effect of these four variables on the benzene entrainer is presented in Figures 4-7.

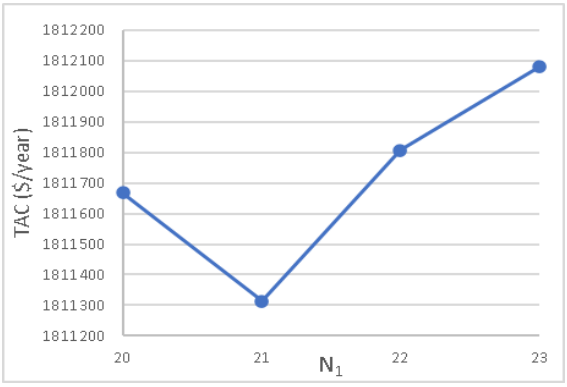

Fig. 4. Effect of N_1 on TAC

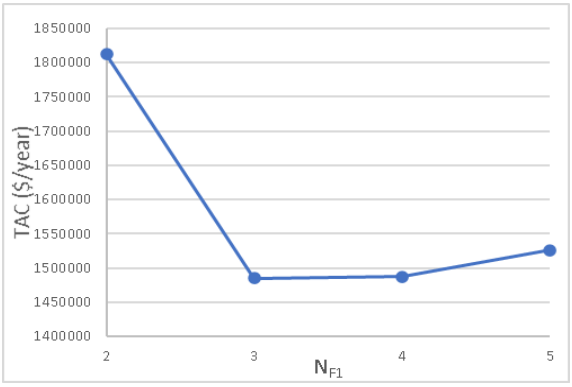

Fig. 5. Effect of N_{F1} on TAC

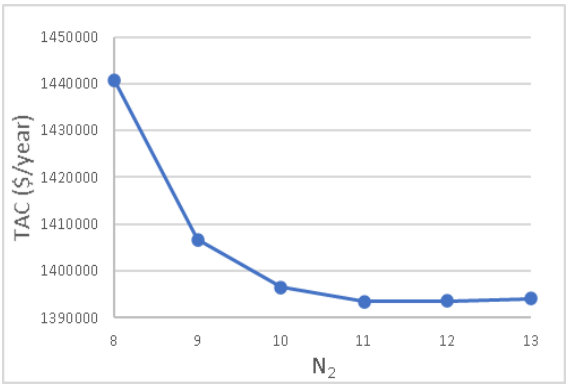

Fig. 6. Effect of N_2 on TAC

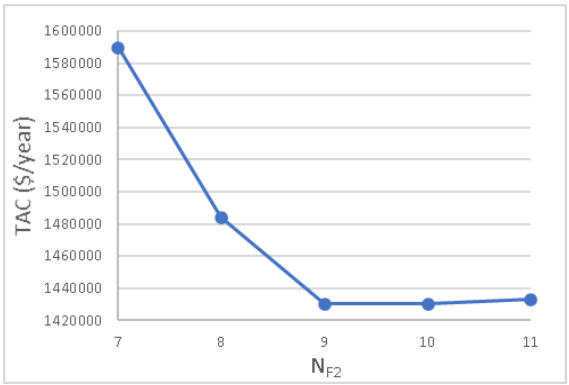

Fig. 7. Effect of N_{F2} on TAC

From Figure 4 to Figure 7 shows that the benzene entrainer has a minimum TAC when N_1 = 21, N_{F1} = 3, N_2 = 11, and N_{F2} = 9. The number of stages of the distillation column will affect both equipment costs and operating (utilities) costs. The larger the number of stages (N_1 and N_2), the higher the equipment costs, but the operating (utilities) costs will be smaller. So several stages produce the lowest TAC. For feed-in locations (N_{F1} and N_{F2}), it does not affect equipment costs but affects operating (utility) costs. The location of the feed that is too close to the reboiler will cause a large reboiler duty. Likewise, the feed that is too upward will increase the load on the condenser.

The cyclohexane entrainer also produced a similar tendency to the benzene entrainer. The comparison of the optimization results between the two entrainers is presented in Table 3.

Table 3. Comparison of Optimization Results

Variable	Entrainer	
	Benzene	***Cyclohexane***
N_1	21	23
N_{F1}	3	7
N_2	11	15
N_{F2}	9	10
TAC	$ 1.430.224 / year	$ 1.637.934 / year

From Table 3, it can be seen that to separate the IPA-water mixture with the same amount and composition and the same product, the benzene entrainer requires less cost than the cyclohexane entrainer. From the research that has been done, the reboiler duty for the benzene entrainer is smaller than the cyclohexane entrainer. This is due to the lower boiling point of benzene compared to cyclohexane. In addition, the dimensions of the distillation column for benzene solvent tend to be smaller than for cyclohexane solvents so that the equipment costs are lower. This could be due to benzene's lower viscosity than cyclohexane, resulting in higher tray efficiency [12].

4. Conclusion

This research obtained the optimum configuration of heterogeneous azeotropic distillation for a mixture of IPA-water with benzene and cyclohexane entrainers. The selection of this entrainer is based on its lightest nature and can form a tertiary azeotrope point in a liquid-liquid phase that a decanter can separate. From the optimization results carried out in stages, the benzene entrainer produces a lower total cost (TAC) than the cyclohexane entrainer. Physical properties such as boiling point and viscosity affect equipment costs and operating costs. An entrainer with a higher boiling point will increase the reboiler load, and an entrainer with a lower viscosity will increase tray efficiency.

References

[1] Collas, F., Kuit, W., Clement, B., Marchal, R., Lopez-Contreras, A. M., and Monot, F. (2012). Simultaneous production of isopropanol, butanol, ethanol and 2,3-butanediol by Clostridium acetobutylicum ATCC 824 engineered Strains. AMB Express 2:45.

[2] J. Pla-Franco, E. Lladosa, S. Loras, and J. B. Montón, "Azeotropic distillation for 1-propanol dehydration with diisopropyl ether as entrainer: Equilibrium data and process simulation", Separation and Purification Technology, 212, pp 692 – 698, 2019.

[3] Arifin S. and I. L. Chien, "Combined preconcentrator/recovery column design for isopropyl alcohol dehydration process", Ind. Engng. Chem. Res., 46, pp 2535–2543, 2007.

[4] Kiss, A. A. (2013). Advanced Distillation Technologies Design, Control and Applications. The Atrium, Southern Gate, Chichester, West Sussex: John Wiley & Sons Ltd.

[5] Smith, R. (2005), Chemical Process Design and Integration, John Wiley and Sons.

[6] J. Meier-Haack, W. Lenk, D. Lehmann, K. Lunkwitz, "Pervaporation separation of water/alcohols mixtures using composite membranes based on polyelectrolyte multilayer assemblies", J. Membr. Sci. 184 (2001) 233.

[7] Luyben, W. L., & Chien, I.-L. Design And Control Of Distillation Systems For Separating Azeotropes. New Jersey: John Wiley and Sons, Inc, 2010.

[8] Chien, I. L.; Zeng, K. L.; Chao, H. Y. "Design and Control of a Complete Heterogeneous Azeotropic Distillation Column System", Ind. Eng. Chem. Res. 2004, 43, 2160.

[9] Ralph Schefflan (2013), Teach Yourself the Basics of Aspen Plus™, John Wiley and Sons.

[10] Wang Y., Peizhe Cui, Yuhong Ma and Zhen Zhang, "Extractive distillation and pressure-swing distillation for THF/ethanol separation", Journal of Chemical Technology and Biotechnology, 90, pp 1463-1472, 2014.

[11] Luyben, W. L. (2006), Distillation Design and Control Using Aspen™ Simulation, John Wiley and Sons, Inc.

[12] R.J. Manivannan, Tony Cai, Ken McCarley, Anand Vennavelli, Sayeed Mohammad, Clint P. Aichele," Point efficiency of sieve trays at elevated liquid viscocities", Chemial Engineering Research and Design, Vol. 159, pp 138 – 145, 2020.