

VOL. 61, 2017



DOI: 10.3303/CET1761265

Guest Editors: Petar S Varbanov, Rongxin Su, Hon Loong Lam, Xia Liu, Jiří J Klemeš Copyright © 2017, AIDIC Servizi S.r.l. **ISBN** 978-88-95608-51-8; **ISSN** 2283-9216

Effect of the Temperature in the Decanter on Total Annual Cost of the Separation Process for Binary Heterogeneous Azeotropic Mixture

Xin Li, Yongkun Wang, Bin Qin, Yinglong Wang, Zhaoyou Zhu*

Qingdao University of Science and Technology, Qingdao, China huagongyl@163.com

Hexane/methanol binary heteroazeotrope was studied to separate by a two-column/decanter process. The mixture was fed to the decanter and layered into two phases whose concentration is changing under various temperatures. Each phase was specified as the feed stream of the two columns so that the costs of the process changed when the decanter temperature are different. Total annual cost (TAC) was used to investigate and optimize the parameters of the process. The minimum TAC was optimized by a sequential iterative optimization procedure. A modified process was developed to further reduce the TAC. The results show that the minimum TAC of the modified process is 4.2 % lower than that of the conventional two-column/decanter process. The operational cost and the capital cost of the modified process are 10.3 % and 2.3 % lower than those of the conventional process. The costs differences under different temperatures demonstrate that the temperature has impacts on the process economics and it should be carefully considered when separating binary heteroazeotropes by the two-column/decanter processe.

1. Introduction

Hexane/methanol binary heteroazeotrope is a common mixture appeared in the pharmaceuticals industry. There are different processes to separate azeotropes such as pressure-swing distillation (Zhu et al., 2015), azeotropic distillation (Yu et al., 2016), and extractive distillation (Wang et al., 2015). Usually, the processes are used to separate homoazeotropes (Rodriguez et al., 2003). But there is a special process that the homoazeotropes are separated by introducing heteroazeotropes. Batch distillation process was applied to separate isopropanol/water mixture by adding benzene as the heterogeneous entrainer (Denes et al., 2009). Ethyl acetate/isooctane mixture was separated by using methanol and acetonitrile (Ooms et al., 2014). Isopropyl alcohol/water binary mixture was separated by adding cyclohexane to form heteroazeotrope with water (Chien et al., 1999). Then the two-column approach was optimized based on TAC (Chien et al., 2004). Ethanol/water binary system was separated through adding benzene to form benzene/water heteroazeotrope (Luyben, 2006). In the above studies, the separation of heteroazeotropes was not further studied. However, the relevant investigations were meaningful (Pirola et al., 2013). Based on the characteristic of layering, a twocolumn/decanter process was proposed to separate the heteroazeotropes (Malone, 2001). N-butanol/water binary mixture was separated by the process. The purities of the products could be stable at 99.9 mol% (Luyben, 2008). A methyl methacrylate separation process with lower operating cost was implemented with a distillation column, a stripping column, and a decanter (Chang and Chien, 2016).

Decanter is an important device for the two-column/decanter process. The heteroazeotropes are layered to two phases in the decanter and each phase is fed into the columns. Under different temperatures, the concentration of the phases is changing so that the costs of the process would vary. However, the published papers didn't study the impact of the decanter temperature on the process economics.

The aim of our paper is to study the economic impact of the decanter temperature on the two-column/decanter process and develop a modified process to implement lower TAC based on the analysis of cold medium in the heat exchangers.

Please cite this article as: Li X., Wang Y., Qin B., Wang Y., Zhu Z., 2017, Effect of the temperature in the decanter on total annual cost of the separation process for binary heterogeneous azeotropic mixture, Chemical Engineering Transactions, 61, 1603-1608 DOI:10.3303/CET1761265

1603

2. Separation feasibility

The two-column/decanter process is shown in Figure 1. The original binary system is fed to the decanter and two phases are appeared. Each phase is fed to the top of the columns and pure products are obtained at the bottom. The vapor from the top is condensed and sent back to the decanter. In Figure 2, the blue dotted line shows the compositions of the main components in the two phases when the decanter temperature is 45 °C and the yellow dotted line shows the compositions when the decanter temperature is 15 °C. It is clear that, with the decrease of the decanter temperature, the composition of hexane in the hexane-riched phase and that of methanol in methanol-riched phase increase. Both the compositions of the two phases are located between azeotropic composition and pure composition within a certain temperature range so it is possible to separate the azeotropic system efficiently. As for the hexane/methanol heteroazeotrope in this paper, the initial binary mixture was fed into the decanter. Then the liquid layered to two phases and each of them was obtained at the top because of the lower boiling point. At the same time, the pure products which are hexane and methanol were respectively obtained at the bottom of each column. Hence, the mixture was separated efficiently by the two-column/decanter process.

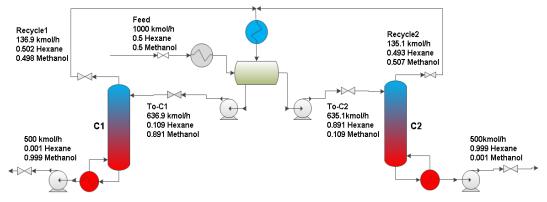


Figure 1: The flowsheet of the two-column/decanter process.

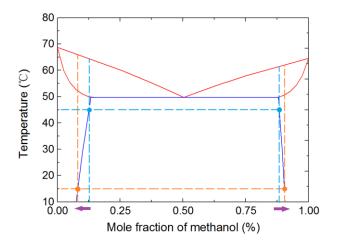


Figure 2: The diagram of the hexane/methanol heteroazeotropic mixture.

3. TAC calculation method

TAC includes operating cost and capital cost. The operating cost consists of annual steam cost and annual cooling water cost while the capital cost contains column vessel cost, plate cost, and heat exchangers cost. The detailed calculation equations have been reported (Zhu et al., 2015). The parameters of the two columns are determined by "tray sizing" function in Aspen Plus. The feed stream is cooled or heated to keep the same temperature with the decanter. The costs of other devices such as pumps, valves, and pipes can be ignored because they are much cheaper. The running time of the process is 8,000 h/y.

1604

4. Design and economic optimization of the processes

Aspen Plus was used to investigate the separation of hexane/methanol heteroazeotropic mixture. The two stripping columns which have individual reboilers were simulated by the "Radfrac" model. Several external condensers were set by using the "HEATER" model. The "DECANTER" model was used as the decanter in the process.

4.1 Optimization procedures

A sequential iterative optimization procedure is applied to minimize the TAC (see Figure 3). The pressures (P1, P2) of the two columns (C1, C2) were 1 atm as well as the decanter. Different decanter temperatures (TD) were studied to minimize the TAC so that the temperature was set as the outer iterative loop parameter. The number of stages in the two striping columns (NT1, NT2) was the inner iterative loop variable. Besides, the bottom product purity was kept at 99.9 mol% by changing the distillate flowrate with the "Design spec/Vary" function.

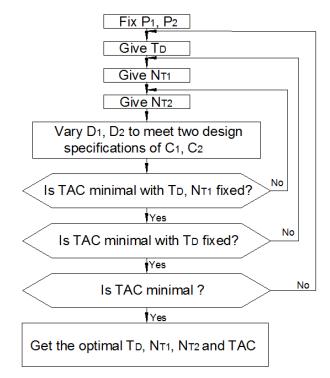


Figure 3: The sequential iterative optimization procedure of the two-column/decanter process.

4.2 Economic analysis

Hexane/methanol heteroazeotrope was separated by the two-column/decanter process with one condenser (see Figure 1). UNIFAC property method (Giuseppe et al., 2014) was used to simulate the process. The feed flowrate of the initial mixture which contains 50 mol% hexane and 50 mol% methanol was set to 1,000 kmol/h at 25 °C. The demands of the bottom product purities were 99.9 mol%. The temperatures of the decanter were changed from 15 °C to 40 °C. It should be noticed that the temperature of the outlet stream from the condenser should be consistent with the decanter as well as the feed stream which was heated or cooled by the heat exchanger. Figure 4 illustrates the results of the process under different decanter temperatures. The minimum TAC is \$1,317,559/y at 35 °C. In the temperature range from 15 °C to 30 °C, the minimum TAC is obtained at 25 °C. But when the temperature increases to 35 °C, a drastic drop occurred. The reason for the drop of TAC at 35 °C is that the cheap cooling water whose initial temperature is 30 °C was used instead of expensive 5 °C refrigerated water. When the temperature of the decanter was lower than 35 °C, the cooling water cannot be applied in the condenser and was replaced by the refrigerated water. The price of the cooling water is 0.354 \$/GJ while that of the refrigerated water is 4.43 \$/GJ so that the price difference influences the TAC. For the operating cost, the trend of the curve is similar. There is a suddenly rise at 35 °C on the capital cost curve because the small temperature differences between the cooling water and the vapor from the columns enlarge the area of the condenser and increase the cost. The price of the cold medium greatly influences the TAC of the process and a modified process which can reduce the impact needs to be developed.

The modified process has two external condensers (Condr1, Condr2) and one cooler (see Figure 5). The cheap cooling water could always be used to condense the vapor from the columns in the condenser while in the cooler, the cooling water and the refrigerated water can be respectively used when the decanter temperature is higher and lower than 35 °C. The combined use of the two cold mediums in the modified process is quite different compared with the use of single cold medium in the two-column/decanter process with one condenser.

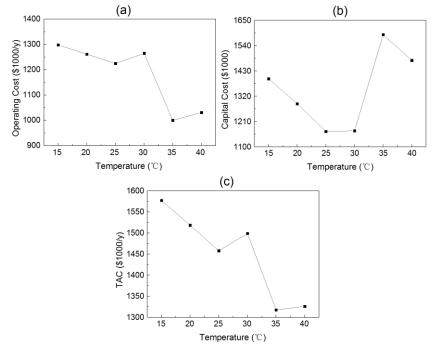


Figure 4: The results of the two-column/decanter process with one condenser.

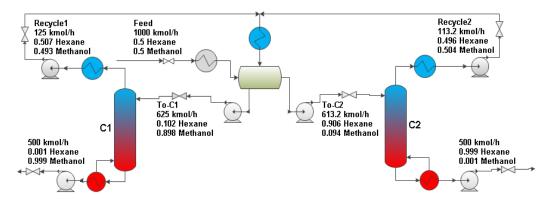


Figure 5: The flowsheet of the modified process.

Figure 6 illustrates the results of the modified process under different decanter temperatures. The minimum TAC is 1,261,678 /y at 25 °C. When the temperature is lower than 25 °C, the TAC decreases consistently. When the temperature is higher than 25 °C, the TAC increases. For the operating cost, the variation tendency is similar. But on the capital cost curve, there is a drop at 40 °C. Because the temperature difference of the outlet stream and the inlet stream in the cooler when the decanter is at 40 °C is larger than that when the decanter is at 35 °C. Therefore, the area of the cooler in the former condition is smaller than that in the latter condition so that the cost is lower at 40 °C.

The results for the two-column/decanter process with one condenser (Process 1) and the modified process (Process 2) were compared (Table 1). The number of stages (NT1, NT2), the column diameters (ID1, ID2), and the costs are shown in Table 1. For the capital costs, the cost is \$1,587,430 in the Process 1 and \$1,424,170 in the Process 2. The cost difference of the two processes is 10.3 %. And for the operating cost,

the cost is \$1,000,070 in the Process 1 and \$976,840 in the Process 2. The cost difference is 2.3 %. As a result, the TAC of Process 2 is 4.2 % lower than that of Process 1.

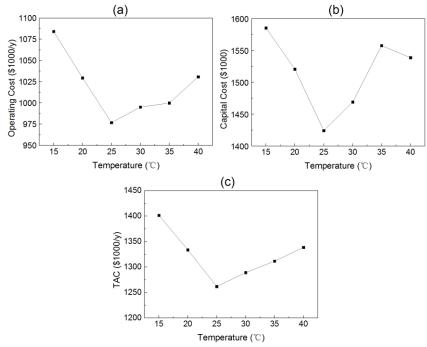


Figure 6: The results of the modified process.

Table 1: The optimal results for the two-column/decanter process with one condenser (Process 1) and the modified process (Process 2) to separate hexane/methanol heteroazeotrope.

Variables	Process 1	Process 2
NT1	7	7
NT2	6	5
ID1 (m)	1.04	1.08
ID2 (m)	1.65	1.68
Capital costs (\$1,000)	1,587.43	1,424.17
Operating costs (\$1,000/y)	1,000.07	976.84
TAC (\$1,000/y)	1,317.56	1,261.68

5. Conclusion

The two-column/decanter process and its modified process were investigated to separate the hexane/methanol heteroazeotropic mixture. It is clearly shown on the diagram that the composition of the layered phases increases with the temperature decreasing. And the phases as the feed streams to the columns further influence the process economics.

TAC was used to optimize the process and it changes with the variation of the decanter temperature. The minimum TAC is \$1,317,559 /y at 35 °C in the two-column/decanter process and is \$1,261,678 /y at 25 °C in the modified process when separating the heteroazeotrope.

The influence of the cost difference between the cooling water and the refrigerated water was reduced by the modified process. Therefore, both the operating costs and the TAC are decreased. The results show that the decanter temperature which is often overlooked has impacts on the economics of the processes and it should be considered carefully when separating the heteroazeotropes.

Acknowledgments

Support from the project of National Natural Science Foundation of China (Project 21676152) is gratefully acknowledged.

References

- Chang W.L., Chien L.L., 2016, Energy-Saving Design and Control of a Methyl Methacrylate Separation Process, Industrial & Engineering Chemistry Research, 55(11), 3064-3074.
- Chien L.L., Wang C.J., Wong D.S.H., 1999, Dynamics and Control of a Heterogeneous Azeotropic Distillation Column: Conventional Control Approach, Industrial & Engineering Chemistry Research, 38(2), 468-478.
- Chien L.L., Kailuen Z.A., Chao H.Y., 2004, Design and Control of a Complete Heterogeneous Azeotropic Distillation Column System, Industrial & Engineering Chemistry Research, 43(9), 760–765.
- Denes F., Lang P., Modla G., Joulia X., 2009, New double column system for heteroazeotropic batch distillation, Computers & Chemical Engineering, 33(10), 1631-1643.
- Giuseppe G., Patricia L., Bart B.S.V., 2014, Separation of methanol tetrahydrofuran mixtures by heteroazeotropic distillation and pervaporation, Aiche Journal, 60(7), 2584-2595.
- Luyben W.L., 2006, Control of a multiunit heterogeneous azeotropic distillation process, Aiche Journal, 52(2), 623-637.
- Luyben W.L., 2008, Control of the Heterogeneous Azeotropic n-Butanol/Water Distillation System, Energy & Fuels, 22(6), 4249-4258.
- Malone M.F., 2001, Conceptual Design of Distillation Systems, Boston, US, ISBN: 0-07-248863-8.
- Ooms T., Vreysen S., Baelen G.V., Gerbaud V.R.D.I., 2014, Separation of ethyl acetate–isooctane mixture by heteroazeotropic batch distillation, Chemical Engineering Research & Design, 92(6), 995–1004.
- Pirola C., Galli F., Bianchi C.L., Carvoli G., 2013, Heterogeneous distillation of the system water-acetic acid-p-Xylene: study of its fluid phase equilibria, micro-pilot column experimental results and computer simulation, Chemical Engineering Transactions, 32, 1897-1902.
- Rodriguez D.I., Gerbaud V., Lelkes Z., Acosta E.J., Papp K., Joulia X., Fonyo Z., 2003, Separation of an azeotropic mixture by heterogeneous extractive continuous distillation, Chemical Engineering Transactions, 3, 355-360.
- Wang Y.L., Zhang Z., Zhao Y.J., Liang S.S., Bu G.L., 2015, Control of Extractive Distillation and Partially Heat-Integrated Pressure-Swing Distillation for Separating Azeotropic Mixture of Ethanol and Tetrahydrofuran, Industrial & Engineering Chemistry Research, 54, 8533-8545.
- Yu H., Ye Q., Xu H., Dai X., Suo X.M., Li R., 2016, Investigation on Thermodynamics in Separation for Ethylene Glycol + Neopentyl Glycol System by Azeotropic Distillation, Journal of Chemical & Engineering Data, 61(7), 2330-2334.
- Zhu Z.Y., Wang L.L., Ma Y.X., Wang W.L., Wang Y.L., 2015, Separating an azeotropic mixture of toluene and ethanol via heat integration pressure swing distillation, Computers & Chemical Engineering, 76, 137-149.