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Comparison of heterogeneous azeotropic distillation and extractive distillation methods for ternary azeotrope ethanol/toluene/water separation

Lei Zhao, Xinyu Lyu, Wencheng Wang, Jun Shan, Tao Qiu *

Jiangsu Key Laboratory of Advanced Catalytic Materials and Technology, School of Petrochemical Engineering, Changzhou University, No.1, Gehu Road, Wujin District, Changzhou, Jiangsu 213164, China

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ABSTRACT

Ethanol and toluene are important organic solvents in chemical industry. Ethanol, toluene and water present a ternary minimum-boiling azeotrope and three binary azeotropes. In this article, two methods are studied to separate the ternary azeotrope: heterogeneous azeotropic distillation using the toluene, which is in the system itself, as entrainer and extractive distillation with glycerol as the only one solvent. In the heterogeneous azeotropic distillation, the pressures of the three columns are changed respectively to achieve heat integration. In the extractive distillation, only one solvent and two columns are used to separate the ternary mixture. Experiment shows that the partially heat-integrated heterogeneous azeotropic distillation reduces the energy cost and total annual cost by 27.7% and 13.4% respectively compared with the conventional heterogeneous azeotropic distillation. Unexpectedly, the extractive distillation can save 18.8% and 39.3% in the energy cost and total annual cost respectively compared with the partially heat-integrated heterogeneous azeotropic distillation.

1. Introduction

Ethanol and toluene are widely used in chemical, pharmaceutical, dye and other fields as good solvents. Ethanol can deliquesce easily and absorb moisture from the air quickly because of the presence of hydrogen bond. Since ethanol, toluene and water present three binary azeotropes and one ternary azeotrope, ordinary distillation methods can not separate the mixture effectively. Some other kinds of distillation methods should be studied to separate the ethanol/toluene/water mixture.

Many methods can be used to separate azeotropic mixture, for example, pressure-swing distillation (Yu et al., 2012), azeotropic distillation (Abu-Eishah and Luyben, 1985), extractive distillation (Meirelles et al., 1992), adsorption (Garg and Ausikaitis, 1983), pervaporation using membrane (Fleming, 1992) and some other new separation techniques. In this article, heterogeneous azeotropic distillation (HAD) and extractive distillation (ED) methods are studied to separate the ethanol/toluene/water mixture.

It is innovative to use toluene, which is in the system itself, as entrainer for the HAD, which will not bring in any other impurities. This special HAD method is applied to separate azeotrope or close-boiling mixtures using the entrainer, which is in the system itself, to generate a lower-boiling azeotrope with the one or two components in the mixture. The minimum-boiling azeotrope produces two immiscible liquid phases in the decanter. Aqueous phase and organic phase both flow back to the column with optimum reflux ratios and the rest are separated and fed into different columns to obtain pure products. HAD for azeotropic mixture is expected to cross the distillation boundary (Doherty and Malone, 2001; Widagdo and Seider, 1996). Kiss used HAD method in bioethanol dehydration with *n*-pentane as entrainer (Kiss et al., 2012). Luyben also used benzene as the entrainer in the separation of ethanol/water azeotrope by HAD (Luyben, 2006a, 2006b).

ED is generally applied to separate binary azeotrope and other close-boiling mixtures with the relative volatility of light components and heavy components below 1.1 (Seader and Henley, 1998; Errico et al., 2013a, 2013b; Kossack et al., 2008; Lei et al., 2003; Liang et al., 2014). The solvent added in the mixture improves the relative volatility of light components and heavy components because the solvent interacts differently with the light components and heavy components in the mixture. When the relative volatility is improved, the light components are acquired in the top of the extractive column (EC) while the heavy components and solvent are acquired from the bottom of the EC for subsequent separation.

* Corresponding author.
E-mail address: qiutao@cczu.edu.cn (T. Qiu).

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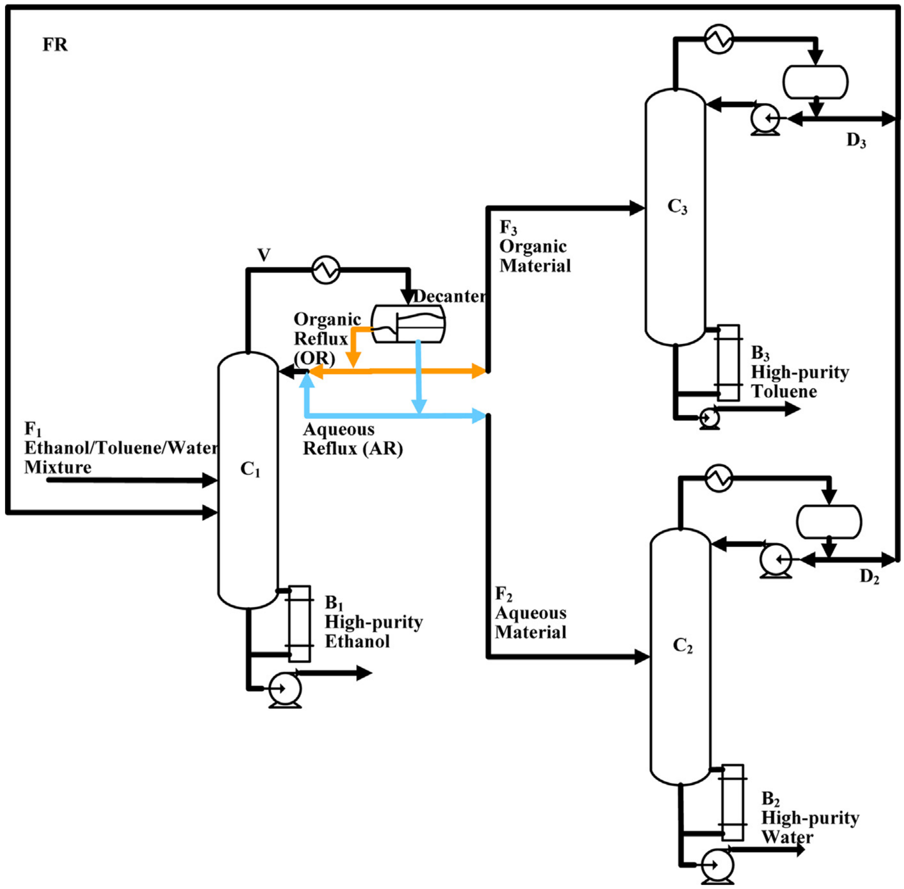

Fig. 1. Process flow sheet of HAD.

Table 1
Azeotropic Temperature and Composition of the System at 1 atm.

Temp (K)	Type	No. Comp.	Toluene (mass%)	Ethanol (mass%)	Water (mass%)
347	Heterogeneous	3	47.49	42.75	9.77
357.68	Heterogeneous	2	80.09	0	19.91
351.3	Homogeneous	2	0	95.62	4.38
350.01	Homogeneous	2	31.92	68.08	0

Solvent and heavy components are separated by a solvent recovery column (SRC) easily. Then, the solvent obtained in the bottom of SRC is recycled to the EC (Kossack et al., 2008). Luyben used dimethyl sulfoxide as solvent to separate maximum-boiling acetone/chloroform mixture by ED (Luyben, 2008). Figueroa used ED method with ionic liquids as solvent to produce anhydrous ethanol and saved energy a lot (Figueroa et al., 2012). Lei used ED method with solid inorganic salt and ionic liquid as solvents to separate ethanol/water mixture (Lei et al., 2014). Long retrofitted conventional ED to a thermally coupled distillation scheme and reduced the energy cost significantly (Duc Long and Lee, 2013).

Separation of the ethanol/toluene/water mixture has visible economic benefit, social benefit and environmental benefit. There are a lot of papers discussing the separation of binary azeotrope via HAD or ED. However, the articles on the separation of ternary azeotrope using HAD and ED are quite limited. So, it is necessary to study some workable distillation methods to separate the ethanol/toluene/water ternary azeotrope, with the emphasis on economic optimization.

In order to separate the ethanol/toluene/water ternary azeotrope, two special distillation methods are studied in this article: HAD and ED methods. According to the total annual cost (TAC), optimization programs are used to get optimal configurations of the two distillation methods.

2. Simulation

2.1. Heterogeneous azeotropic distillation

2.1.1. Process design and ternary diagrams

In the separation of the ternary mixture with ethanol/toluene/water, the toluene can also serve as an entrainer and form a low-boiling ternary azeotrope with ethanol and water. So, it does not need to add any other entrainer, which will not bring in any other impurities. The ethanol/toluene/water mixture presents three binary azeotropes and one ternary azeotrope. One ternary azeotrope (ethanol/toluene/water) is satisfactory because it is heterogeneous and its azeotropic temperature (347 K) is the lowest in the system. Another three binary azeotropes are also formed with azeotropic temperatures of 357.68, 351.3 and 350.01 K, respectively. Table 1 shows the azeotropic temperature and composition of ethanol/toluene/water mixture at 1 atm. When the pressure is 2.18 atm or 0.33 atm, the ternary azeotrope is still heterogeneous and its azeotropic temperature is still the lowest in the system. The NRTL physical property model is used in the simulation for the separation of the ternary azeotrope.