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SIMULATION OF PRESSURE-SWING DISTILLATION FOR SEPARATION OF ETHYLENE GLYCOL AND 1,2-BUTANDIOL

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ABSTRACT

A pressure-swing distillation process for separation of ethylene glycol and 1,2-butandiol is proposed on the basis of characteristic analysis on the ethylene glycol-1,2-butandiol azeotropic system. Simulation is performed by using Aspen Plus simulation software, aiming at minimizing the energy consumption and guaranteeing the concentrations of ethylene glycol and 1,2-butandiol products. The influences of total number of theoretical plate, reflux ratio, feeding position and other parameters on the separation efficiency are specified. The optimal process parameters for the atmospheric distillation column are as follows: the operating pressure is 100kPa, the number of theoretical plate is 45, the feeding position is between the 30-40th plate, and the reflux ratio is 7. The optimal process parameters for the vacuum distillation column are as follows: the operating pressure is 30kPa, the number of theoretical plate is 50, the feeding position is at the 20-40th plate, the reflux ratio is 4. Under the optimal parameters, the mass purity of ethylene glycol and 1,2-butandiol products exceed 99% and 98%, respectively, which meets industrial production requirements

KEYWORDS

Ethylene glycol,1,2-butandiol, pressure-swing distillation, simulation.

1. INTRODUCTION

In recent years, with the development of polyester industry, the demand for ethylene glycol is increasing year by year [1-3]. In China as an oil-poor country, the use of petroleum as a raw material to produce ethylene glycol (EG) is not preferable. Therefore, the use of coal or biomass to make ethylene glycol has gradually been concerned. However, it is also difficult to separate ethylene glycol completely from other alcohols using general separation methods [4]. At present, in the process of producing ethylene glycol from biomass, the components in the obtained chemical alcohol are commonly complex [5]. After the initial separation, a mixture containing ethylene glycol, propylene glycol and a series of butanediol mixtures is obtained. Moreover, a binary compound comprising of EG and 1,2-butandiol (1,2-BD) is inevitably received in the following product-separation process [6]. For instance, in the process of catalytic hydrogenation for dimethyl oxalate, it will produce 1,2-BD and other side products due to the excessive hydrogenation of dimethyl oxalate. At ambient temperature, EG and 1,2-BD are mutually soluble, both boiling points are very closer, and form a binary azeotropic system, so that there has been an effective method to separate the mixture until now [7-9]. In this article, a process of pressure-swing distillation is suggested to separate the azeotrope of EG and 1,2-BD, and Aspen Plus soft is applied to simulating the separation process, for meeting the purity and recovery of the both products, the optimum process conditions is expected to be accepted, which provides a feasible separation process for the separation of EG-1,2-BD azeotrope [10,11].

2. SIMULATION OF SEPARATION PROCESS

2.1 Objective of Separation

The amount of raw material separated is set to be 1000 kg/h, contains 80wt% of EG and 20wt% of 1,2-BD. The feed temperature is 40°C, after separation, the purity of EG and 1,2-BD is above 99wt% and 98wt%, respectively.

2.2 Selection of thermodynamic model

EG-1,2-BD is a non-ideal binary system, and the mixture is inter-miscible, different thermodynamic models in Aspen Plus software are selected to calculate the azeotrope properties of EG-1,2-BD binary system. However, the phase equilibrium data for the binary system in Aspen Plus is insufficient. In the case of it, reference of vapor-liquid phase equilibrium for the EG-1,2-BD system become very important. In this process simulation, NRTL (non-random two liquid) model was employed, and model parameters suited were obtained from the previous references which acquired from thermodynamic experiments in EG-1,2-BD binary system at different pressures.

2.3 Feasibility of separation process

The vapor-liquid phase equilibrium data of EG-1,2-BD system under different pressures were regressed using NRTL model by Aspen Plus simulation soft, on the basis of verification through thermodynamic consistency test, binary interaction parameters were obtained, and induced into the Aspen Plus simulation database. After that, x-y diagram representative for liquid and liquid compositions at 30kPa and 100kPa, respectively, were calculated and described below. As shown in Figure 1, the lowest azeotrope temperature point at 30kPa and 100kPa pressures is shown in the binary system of EG and 1,2-BD, with azeotrope composition of EG varying from 0.3 to 0.43, respectively. Therefore, it is feasible to simulate the separation between EG and 1,2-BD using Aspen Plus software by adjusting operation pressure.

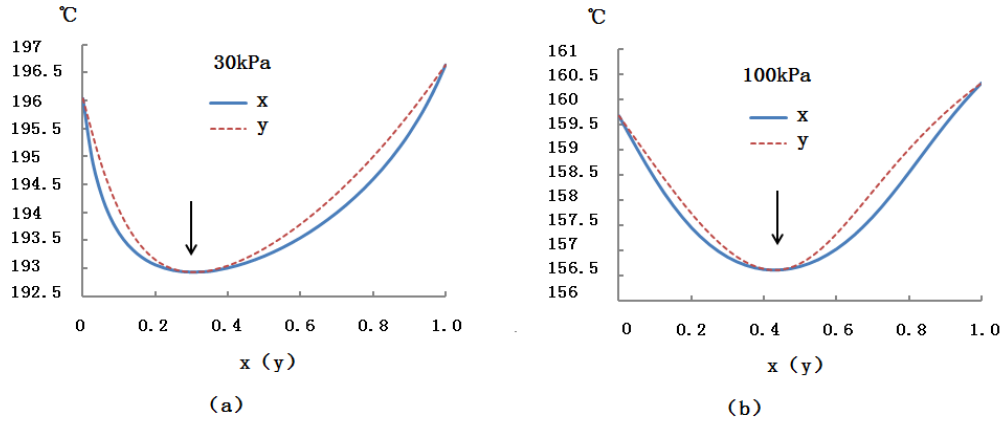

Figure 1: Diagram of vapor-liquid phase equilibrium for EG-1,2-BD binary system at different pressure: (a) 30kPa, (b) 100kPa

2.4 Establishment of separation sequence

A process of pressure-swing distillation was established for the EG-1,2-BD mixture. The process is composed of an atmospheric column (T1) and a vacuum column (T2). A raw material mixture(F) enters T1, an overhead distillate on the top of the column is withdrawn in the form of EG-1,2-BD azeotrope(D1), and a flow of EG with higher purity(W1) is harvested. In the meantime, the flow of D1 is introduced into T2, in which another azeotrope of EG-1,2-BD is received from the top of T2and returned to T1, and pure 1,2-BD product is retained on the bottom of T2. The process diagram is shown in Figure 2.

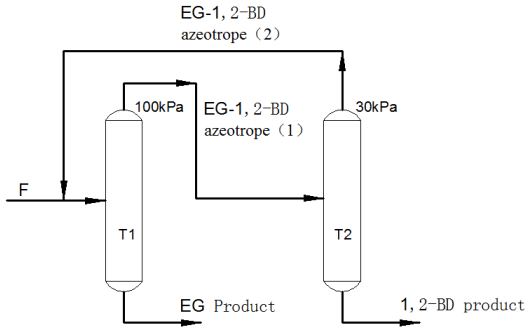

Figure 2. Process diagram for separation EG and 1,2-BD by pressure-swing distillation

2.5 Process Simulation

First, DSTWU model in Aspen Plus software was used to complete the simple calculation of T1 and T2 for the given separation objective, obtaining the design parameters including calculated theoretical plate number, minimum reflux ratio and feed position. Based on the data of parameters, RadFrac model in Aspen Plus software was employed to complete the detailed calculation of T1 and T2, to carry on DesignSpecs accounting, to ensure that products meet the separation requirements of productions. Finally, the Sensitivity analysis tool was adopted, the purity of EG and 1,2-BD was set to be the constraint variable, the minimum energy consumption was seen to be the objective function, the optimization of process parameters of each distillation column was completed.

3. RESULTS AND DISCUSSION

3.1 Influence of the variation of the number of theoretical plates on the separation effect

On the basis of the invariant of other simulated conditions, the influence of the change of the theoretical plate number of the ambient pressure column and the vacuum pressure column on the purity of the column kettle product and the energy consumption of the reboiler were investigated respectively.

As shown in the figure 3, with the increase of the theoretical plate number, the purity of the column kettle product of T1 and T2 increases gradually. When the number of theoretical plate of T1 is over 45, and that of T2 is greater than 50, the purity is basically unchanged. On the other hand, with the increase of the theoretical tray number, the energy consumption of the reboiler shows the same change trend, and also be much constant at 45th and 50th theoretical plate. Therefore, the theoretical plate number of high pressure tower and low-pressure tower is 45 and 50 respectively.

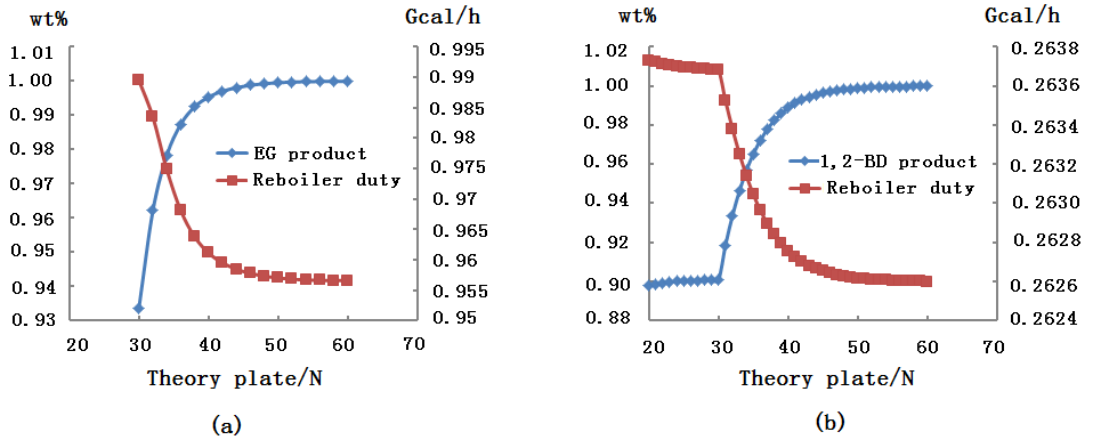

Figure 3: Effect of theory plate number on product composition and reboiler duty: (a) column T1, (b) column T2

3.2 Influence of the variation of feed position on the separation effect

On the basis of the invariant of other simulated conditions, the effects of the feeding position of the ambient pressure column and the vacuum pressure column on the purity of the column kettle product and the energy consumption of the reboiler were investigated.

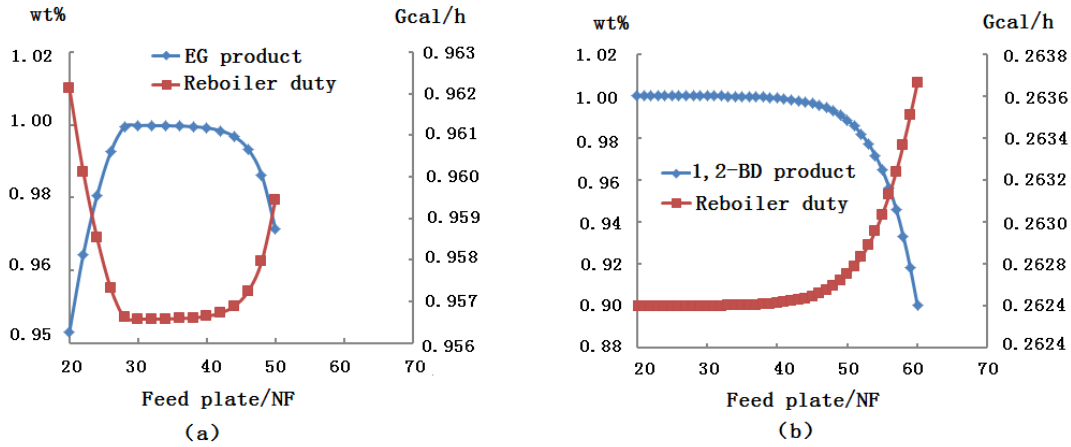

Figure 4: Effect of feed plate number on product composition and reboiler duty: (a) column T1, (b) column T2

As shown in the figure 5, for the ambient pressure column T1, both the concentration of the column kettle product EG and the energy consumption of reboiler are almost unchanged at the position of feed plate ranging from 27 to 40. However, except from the feed interval, either the purity of EG decreases or the reboiler duty increases. For the vacuum pressure column, both the purity of 1,2-BD and the energy consumption of the reboiler all keep constant among the number of feed plate ranging from 20 to 45, nevertheless. When the feed position is moved down more than 45th plates, the purity of the tower kettle product is gradually reduced, because a certain amount of material enters the tower kettle leading to the decrease of the purity of the tower kettle product. At the same time, the energy consumption of the reboiler of the vacuum column increases sharply. Therefore, the preferable position of feed is controlled between 30 and 40 for the column T1, and between 20 to 40 for the column T2, respectively.

3.3 Influence of the variety of reflux ratio on the separation effect

Reflux ratio is one of the main conditions to ensure continuous and stable operation of rectification column. On the basis of the invariant of other simulated conditions, the influence of reflux radio of the ambient pressure column and the vacuum pressure column on the purity of the tower kettle product and the energy consumption of the reboiler were investigated respectively.

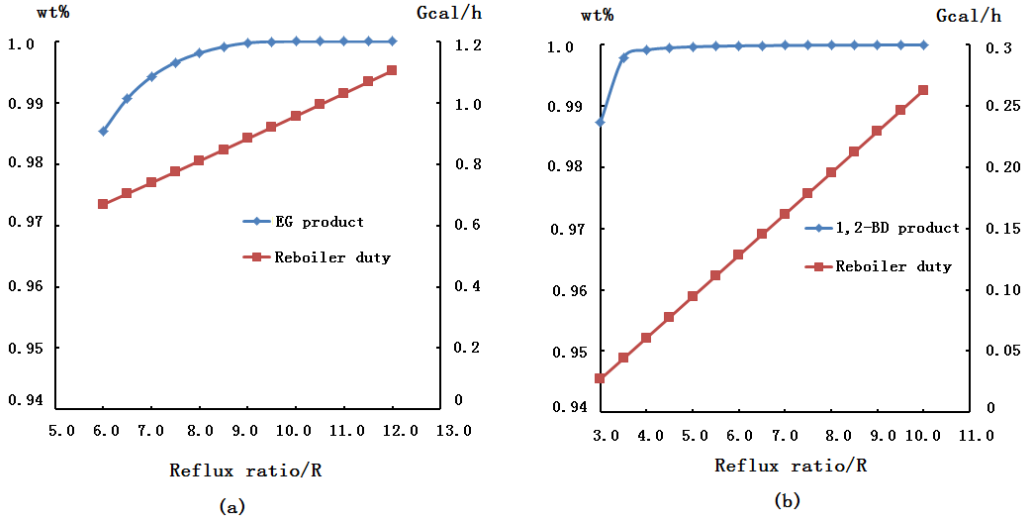

Figure 5: Effect of reflux ratio on product composition and reboiler duty: (a) column T1, (b) column T2

As shown in the figure 5, with the increase of reflux radio, the purify of the tower kettle product of column T1 and columnT2 rises gradually and then to be constant. The energy consumption of the reboiler in the both cases increases linearly with the increment of reflux ratio, which indicates that the energy consumption of reboiler is positively correlated with the reflux ratio. Considering the requirement of separation and energy consumption, the suitable reflux ratio of the both column is 7 and 4, respectively.

3.4 Optimization of process parameters

The above method is used to simulate the process parameters, and the optimized parameters are shown in table 1.

Table 1: Optimal parameters of process simulation

Distillation	Operation pressure/kPa	Number of Theoritical plate	position of Feed plate	Reflux ratio
T1	100	45	30-40	7.0
T2	30	50	20-40	4.0

Based on the process parameters in table 1, the distillation for separating EG and 1,2-BD by pressure-swing method was simulated sequentially in a steady state. For the column T1, the EG product was obtained at the column kettle with the purity being above 0.99wt%. For the column T2 receiving the azeotropic mixture of EG and 1,2-BD as feedstock, 1,2-BD product was concentrated on the bottom, the purity of 1,2-BD reached at 0.98wt%. It can be seen that the effective separation of EG and 1,2-BD can be achieved by using the pressure-swing distillation process.

4. CONCLUSION

Based on the characteristics of EG-1,2-BD azeotrope system, a pressure-swing distillation process for separating EG and 1,2-BD was established. Aspen plus simulation software was used to analyze and optimize the process. The mass fraction of EG and 1,2-BD products was not less than 99wt% and 98wt%, respectively. The achieved process provides a theoretical basis for engineering research.

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