

## Separation technology for methanol-toluene system by double column distillation

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### Abstract

In this paper, Computer has been used to simulate the pressure-swing distillation process for separating the mixture of methanol and toluene. The Wilson activity model is chosen as the property package in the simulation using the built-in binary interaction parameters in the simulator. Through the analysis to the y-x curves of methanol and toluene predicted by Wilson under the pressure of 0.1 and 0.5 MPa, the feasibility of separation was found. Aspen Plus was used to simulate and optimize the whole process, and the optimal process parameters were determined. Under the optimal condition, the results showed that the mass fraction of methanol and toluene were both 99.5%.

### Keywords

Pressure-swing distillation, Methanol, Toluene.

### 1. Introduction

Both methanol and toluene are widely used as organic solvents in medicine, fine chemical industries and other fields[1,2]. However, as the formation of methanol-toluene azeotrope, it is a challenging task to separate the two components. Some special processes, such as pervaporation process[3,4], extractive distillation[5,6] and pressure-swing distillation[7] have been used to separate such azeotropes or close-boiling mixtures.

For pervaporation process, high operating costs and technical difficulties are the two main factors of restricting its industrialization. For extractive distillation, the volatilities of components to be separated are altered by using an additional component, which also increases the cost of recycling and adding extraction agent[8]. Compared with those two processes, pressure-swing distillation based on the principle that the azeotropic composition can vary considerably by changing the pressure will make separation easier[9].

### 2. Separation Scheme

In this paper, Computer has been used to simulate the pressure-swing distillation process for separating the mixture of methanol and toluene. The feed is a mixture made up of 72.2 wt% methanol and 27.8 wt% toluene, with a mass flow rate of 1000 kg/h. The molar ratios of top to feed in distillation towers are automatically adjusted through the Design Specs/Vary function, which controls the mass fraction of products (99.5 wt% methanol and 99.5 wt% toluene). Then the main parameters such as stage number, reflux ratio and feed position are optimized in this study.

#### 2.1 Vapor Liquid Equilibrium

The Wilson activity model is chosen as the property package in the simulation using the built-in binary interaction parameters in the simulator. Figure 1 illustrates the y-x curves of methanol and toluene predicted by Wilson under the pressure of 0.1 and 0.5 MPa. Methanol-toluene is the maximum-boiling system, while the mass fraction will be varied from 72.2 wt% methanol and 27.8 wt% toluene at 0.1 MPa to 84.0 wt% methanol and 16.0 wt% toluene at 0.5 MPa. Thus, this dramatic change can carry out the separation of methanol-toluene.

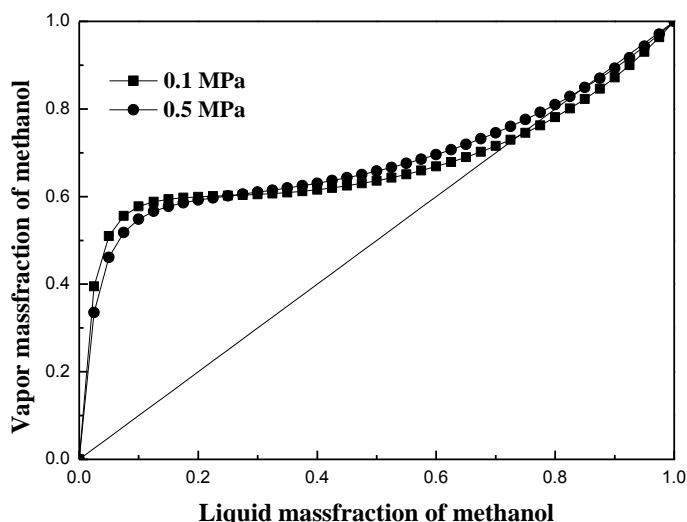


Figure 1. The y-x curves of methanol-toluene at 0.1 and 0.5 MPa

### 2.2 Pressure-swing Distillation Design

The original mixture will be separated into toluene product and high-pressure light liquid phase that the main composition is methanol through pressurized tower. Then, the high-pressure light liquid phase will be separated into methanol product and atmospheric pressure light liquid phase through atmospheric tower. Stream Feed, PD1 and PD2 is the feed stream, toluene product and methanol product respectively, while both TOWER1 (pressurized tower) and TOWER2 (atmospheric tower) select RadFrac model, the mixer uses the Mixer model and booster pumper selects Pump model.

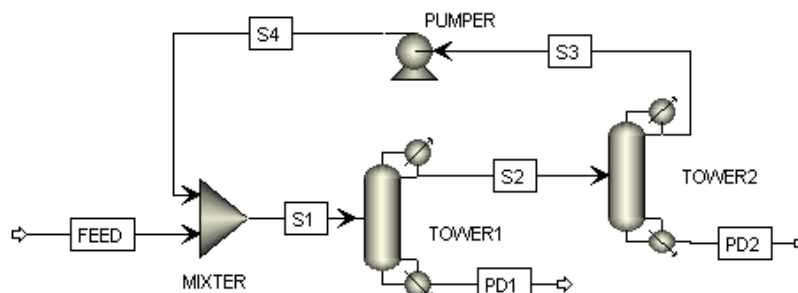


Figure 2. Flowsheet for the pressure-swing distillation process

## 3. Process Simulation and Optimization

### 3.1 Optimization of Stage Number

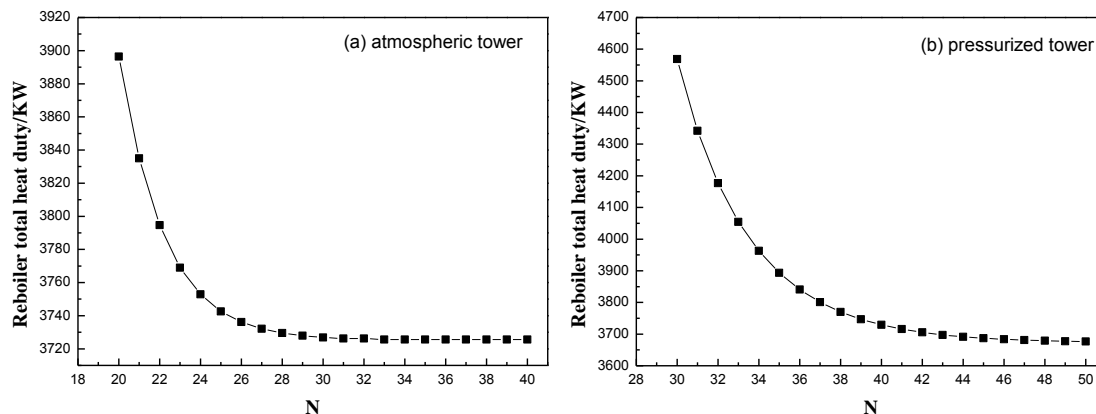


Figure 3. The effect of the theoretical stage number on the reboiler total heat duty

The effect of theoretical stage number on the reboiler total heat duty of pressurized and atmospheric tower is shown in Figure 3. The shifts in the heat duty with stage number are clearly seen from Figure

3. It indicates that under the premise of ensuring the degree of separation, the reboiler total heat duty has a significant decline in a certain range. Owing to the increased equipment costs with the increasement of theoretical stage number, the number of theoretical stages of pressurized tower is selected 28, and the number of theoretical stages of atmospheric tower is selected 40.

### 3.2 Optimization of Feed Position

The effect of different feed stages on the reboiled heat duty of pressurized and atmospheric tower is shown in Figure 4. It can be seen that as the feed stage moves from the top to the bottom, the reboiler total heat duty reduces first and then increases. When the feed stage of pressurized and atmospheric tower is 20 and 12, the reboiler total heat duty is the lowest as illustrated in figure 4, thus the feed stage of pressurized tower is selected 20, and the feed stage of atmospheric tower is chosen 12.

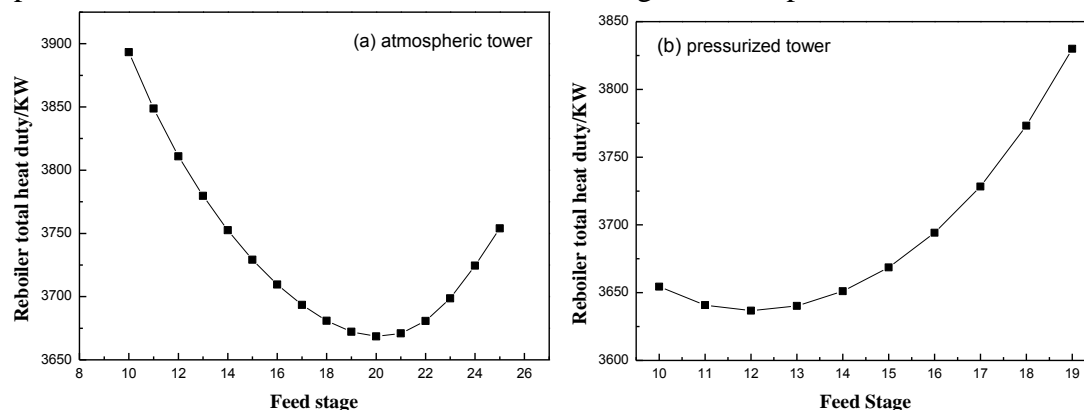


Figure 4. The effect of the feed stage on the reboiler total heat duty

### 3.3 Optimization of Reflux Ratio

The reboiler total heat duty reduces rapidly first and increases quickly with the increasement of reflux ratio as shown in Figure 5. In Figure 5(a), when the reflux ratio of pressurized tower reaches 1.8, the reboiler total heat duty reaches the lowest, so the optimal reflux ratio of pressurized tower is 1.8. In the same way, the simulation results from Figure 5(b) shows that the optimal reflux ratio of atmospheric tower is 2.6.

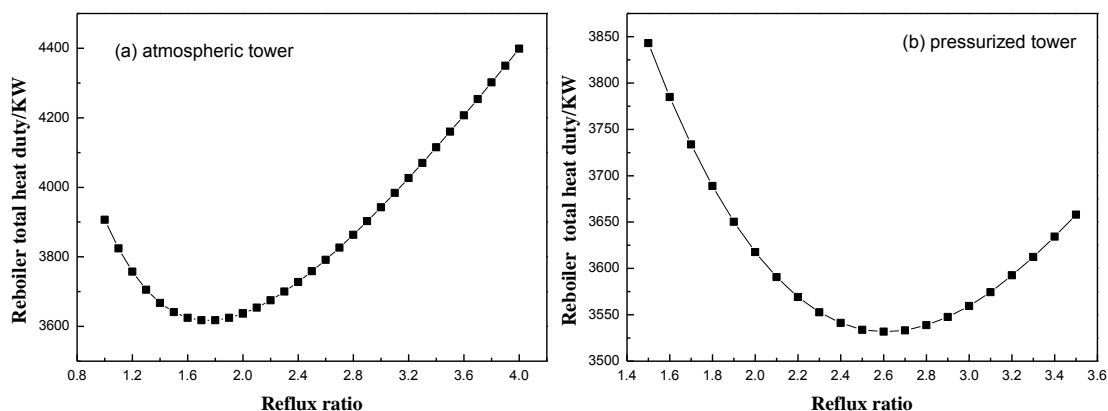


Figure 5. The effect of the reflux ratio on the reboiler total heat duty

### 3.4 Results in Optimum Parameters

Table 1 shows the optimum parameters of the pressure-swing distillation for methanol-toluene.

Table 1 optimum parameters of the pressure-swing distillation for methanol-toluene.

Tower	Stage number	Reflux ratio	Feed stage	Pressure
Pressurized tower	28	1.8	20	0.1 MPa
Atmospheric tower	40	2.6	12	0.5 MPa

The simulation results are shown in Table 2 according to the above optimum parameters.

Table 2 Simulating results under optimum parameters

	Feed Stage	Pressurized tower		Atmospheric tower	
		Top	Bottom	Top	Bottom
Temperature/°C	30	111.3	166.1	63.9	70.7
Pressure/MPa	0.6	0.5	0.5	0.1	0.1
Mass fraction/%					
Toluene	72.2	18.1	99.5	24.8	0.5
Methanol	27.8	81.9	0.5	75.2	99.5

#### 4. Conclusion

The Paper proposed a separation method for the azeotrope of methanol-toluene. Firstly, through the analysis to the y-x curves of methanol and toluene predicted by Wilson under the pressure of 0.1 and 0.5 MPa the feasibility of separation was found. Then the binary azeotrope of methanol and toluene was separated by pressure-swing distillation. Aspen Plus was used to simulate and optimize the whole process, and the optimal process parameters were determined. Under the optimal condition, the results showed that the mass fraction of methanol and toluene were both 99.5 %.

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#### References

- [1] Y.D. Ji, B. Zhang, K. Zhang: Core/shell-Structured ZSM-5@Mesoporous Silica Composites for Shape-Selective Alkylation of Toluene with Methanol, *Acta Chimica Sinica*, Vol. 71(2013) No.3, p. 371-380.
- [2] L.L. Li, M. Janik, X.W. Nie: Reaction Mechanism of Toluene Methylation with Dimethyl Carbonate or Methanol Catalyzed by H-ZSM-5, *Acta Physico-Chimica Sinica*, Vol. 29(2013) No.7, p. 1467-1478.
- [3] N.R. Singha, S.B. Kuila, P: Separation of toluene-methanol mixtures by pervaporation using crosslink IPN membranes, *Chemical Engineering and Processing*, Vol. 48(2009) No.11, p. 1560-1565.
- [4] P. Garg, R.P. Singh, V. Choudhary: Selective polydimethylsiloxane/polyimide blended IPN pervaporation membrane for methanol/toluene azeotrope separation, *Separation and Purification Technology*, Vol. 76(2011) No.3, p. 407-418.
- [5] D.M. Yang, P. Ye, M.F. Ye: Separation of methanol-toluene by combined process of extraction with salt and distillation, *Chemical Engineering(China)*, Vol. 42(2014) No.5, p. 31-34.
- [6] C.Y. Zhang, C.Z. Zheng, J.H. Tang: Process Simulation of Extractive Distillation for Methylcyclohexane and Toluene System, *Petrochemical Technology*, Vol. 40(2011) No.5, p. 532-535.
- [7] Z.Y. Zhao, D.F. Xu, X.Z. Liu: Separation of acetonitrile /methanol/ benzene ternary azeotrope via triple column pressure-swing distillation, *Separation and Purification Technology*, Vol. 169(2016) No.6, p. 66-77.
- [8] J. Lee, J. Cho, D.M. Kim Dong-min: Separation of tetrahydrofuran and water using pressure swing distillation: Modeling and optimization, *Korean journal of Chemical Engineering*, Vol. 28(2011) No.2, p. 591-596.

- [9] Y.J. Gao, J.J. Hu, H. Jia: Comparison of pressure-swing distillation and extractive distillation with varied-diameter column in economics and dynamic control, *Journal of Process Control*, Vol.49(2017) No.1, p. 9-25.