Energy-Efficient Vacuum-Distillation Process for Separating Diluted Acetonitrile-Water Mixture: Rigorous Design with Experimental Verificationfrom Ternary Liquid-Liquid Equilibrium Data

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Abstract:

According to the feature that composition of the Azeotrop could be changed with the change of pressure, the method of pressure-swing distillation was applied to separate the azeotrope of acetonitrile-water and obtain high purity acetonitrile. A simulation model of pressure-swing distillation system was established by chemical engineering software Aspen Plus to get initial results. Meanwhile, the influence of process parameters such as reflux ratio, feed stage, tower pressure and distillate flow rate on the rectification effect was analyzed by the model analysis tools. Ultimately, the optimization model of minimum energy consumption of distillation process was established under the premise assuring the quality of products to obtain energy- efficient optimizing operation parameters. The results showed that the simulation met technology requirements, saved energy 25% and laid the foundation for design and implementation of real-time optimization control system.

Keywords-acetonitrile; pressure-swing distillation; simulation; optimization

Introduction:

Acetonitrile is widely used in organic synthesis as an intermediate reagent, solvent, azeotropizer 1-2 and in highly effective liquid chromatography a mobile phase therefore the investigation and development of inexpensive and commercially convenient methods for acetonitrile production represent an urgent problem. Some special techniques should be used to obtain the high purity acetonitrile while water and acetonitrile are apt to form an azeotrope. At present, the main methods to separate acetonitrile from the acetonitrile-water azeotrope are pressure-swing distillation, Azeotropic distillation, salt fractionation, dehydration, extractive distillation, interval salting extractive distillation. In petrochemical industry, according to the feature that composition of the azeotrope could be changed with the change of pressure, the method of pressure-swing distillation was usually applied to separate the azeotrope of acetonitrile-water and obtain high purity acetonitrile [1, 4]. Aspen Plus is a large-scale chemical engineering process software, based on steady state chemical engineering simulation, optimization, sensitivity analysis and economic evaluation, providing a set of intact unit operation model, and used for various operation process. From single operation to the whole process simulation, it also is the only complex process simulation system in the world that can solve problems of complicated materials like solid, electrolyte, biomass, routine materials and the like. Its applications in calculation of phase equilibrium and distillation of multiple towers give expression to the important development of modern process technology development level [5, 7].

Pressure-swing distillation process of acetonitrile-water was simulated by Aspen Plus process simulation software in this study, whose sensitivity analysis tool was used to analyst the influence of operating parameters to production. Meanwhile, the optimization model of minimal energy consumption of distillation process was established and the best operating parameters were obtained, which has an important guiding significance to the experiment.

I. PROCESS AND SEPARATION PRINCIPLE OF PRESSURE-SWINGDISTILLATION:

A) Separation Principle

As we know, the mass composition of acetonitrile-water azeotrope is 84% acetonitrile and its azeotropic point is 77℃ under atmospheric pressure. According to the composition curves (FIGURE I & FIGURE II) of acetonitrile in the azeotrope of acetonitrile-water under different pressure, at 0.4bar, the mass fraction of acetonitrile is 0.87, and at 3.5bar, it becomes 0.76. On the basis of the feature that composition of the azeotrope could be changed with the change ofpressure, the method of pressure-swing distillation could be used to obtain the high purity acetonitrile.

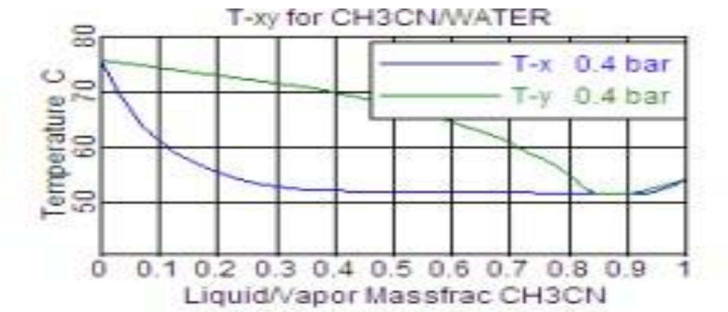

FIGURE I. P=0.4BAR, T-X-Y CURVE OF ACETONITRILE-WATER AZEOTROPE

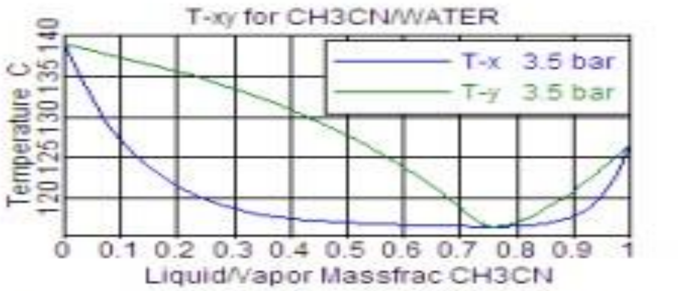

FIGURE II. P=3.5BAR, T-X-Y CURVE OF ACETONITRILE-WATER AZEOTROPE

B) Process Description:

The FIGURE III shows the process of pressure-swing distillation that consists of vacuum tower (B1) and pressurized rectifying tower (B2) under different operating pressure. PUMP is a booster pump connecting the vacuum tower and the pressurized tower, 1-RAW-IN is raw stream, 3-REC-O is the circular stream, 2-WAT-O is the stream from vacuum tower kettle (waste water), and 6-PROD-O is the final product acetonitrile stream

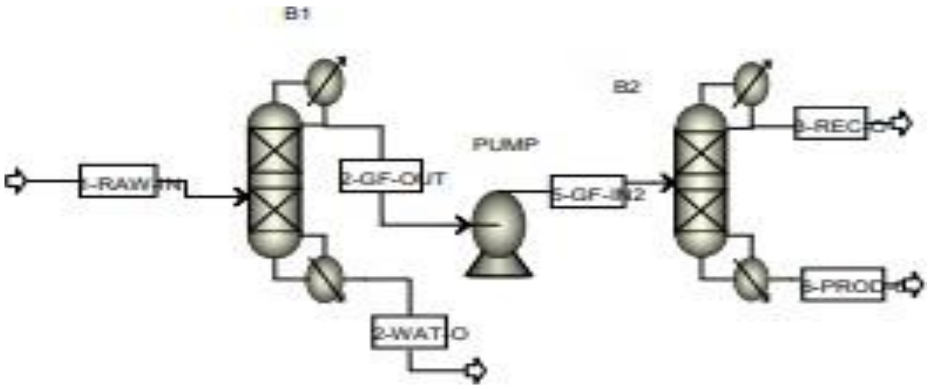

FIGURE III. THE FLOW DIAGRAM OF ACETONITRILE-WATER PRESSURE- SWING DISTILLATION PROCESS

In which, acetonitrile-water stream (1-RAW-IN) and the liquid phase stream (3-REC-O) from the top of the pressurized tower needed to separate ulteriorly were mixed up and got access to Tower B1, where stream (2-WAT-O) from the bottom was mostly water, and the stream (2- GF-OUT) was the acetonitrile-water azeotrope, which turned to stream (5-GF-IN2) and as the feed of pressurized tower by the booster pump (PUMP), thus, the stream (6-PRO-O) was obtained from the bottom of pressure tower was the high purity acetonitrile

II. System Simulation:

A. Process Requirements:

In accordance with the separation results, the feed composition was approximately 50% acetonitrile and 50% water (mass fraction), quantity of flow was 100Kg/h. According to the actual production, the mass fraction of water in the azeotrope from the top of vacuum tower should be controlled less than 13%, and the mass fraction of water from the top of pressure tower should be more than 24%. Thus, the high purity acetonitrile (99.9%) could be obtained from the bottom of pressurized tower, and the mass fraction of water could be less than 50ppm

B. Simulation Calculation

The initial simulation was carried out with parameters as the TABLE I. Then, the pressure- swing distillation process was calculated by NRTL model and Radfrac modules, whose results as TABLE II. The purity of product acetonitrile was over 99.9% and water fraction was less than 50ppm, which was satisfied the separation requirement. However, the reboilers and condensers of the two towers were of high duty. So, on the basis of separating effect, energy reduction was needed and the initial operating parameters should be optimized.

TABLE I. THE INITIAL PARAMETERS OF DISTILLATION TOWERS

Column	The initial parameter of distillation tower			
	Reflux ratio	Temperature (^{0}C)	Feed position	Total stages
Vacuum tower	2.0	0.5	14	20
pressurized tower	3.0	3.5	14	20

TABLE II. THE INITIAL OPTIMIZED RESULTS OF DISTILLATION TOWERS

Column	The initial parameter of distillation tower							
	Stream	Temperature ^0C	Pressure /bar	Acetonitrile mass fraction w%	Moisture mass fraction	Mass flow	Heat duty mmkcal/hr	
Vacuum tower	1-RAW-IN	25.0	1.00	0.5000	0.5000	100.00	TOP	-0.03982
	2-GF-OUT	51.5	0.40	0.8706	0.1294	57.00		
	2-WAT-O	75.9	0.40	32ppm	1.000	42.568	KETTLE	0.04249
Pressurized tower	5-GF-IN2	52.1	4.00	0.8706	0.1294	57.432	TOP	-0.03062
	3-REC-O	116.5	3.50	0.7612	0.2388	31.121		
	6-PROD-O	126.6	3.50	1.000	45ppm	26.311	KETTLE	0.03341

III. SENSITIVITY ANALYSIS:

A.Sensitivity Analysis of Vacuum Tower:

Where, the influence of process parameters such as reflux ratio-R, feed stage-NF, tower pressure-P and distillate flow rate-D on the rectification effect of vacuum tower was analyzed by the model analysis tools. Sensitivity analysis of R is shown in FIGURE IV, NF is shown in FIGURE V, P is shown in FIGURE VI, and D is shown in FIGURE VII. Results showed that the R should be more than 1.6, the NF should be in the range of 14 to 17, the P should be less than 0.4 bar, and the D should be less than 57 kg/hr.

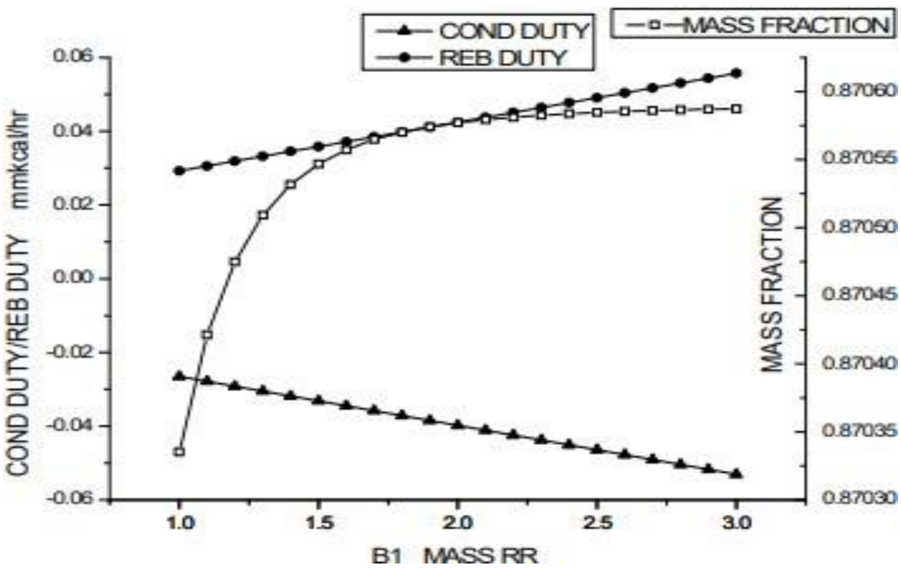

Figure Iv. The Effect Of Reflux Ratio On Mass Fraction Of Acetonitrile, Heat Duty Of Reboiler And Condenser In Vacuum Tower.

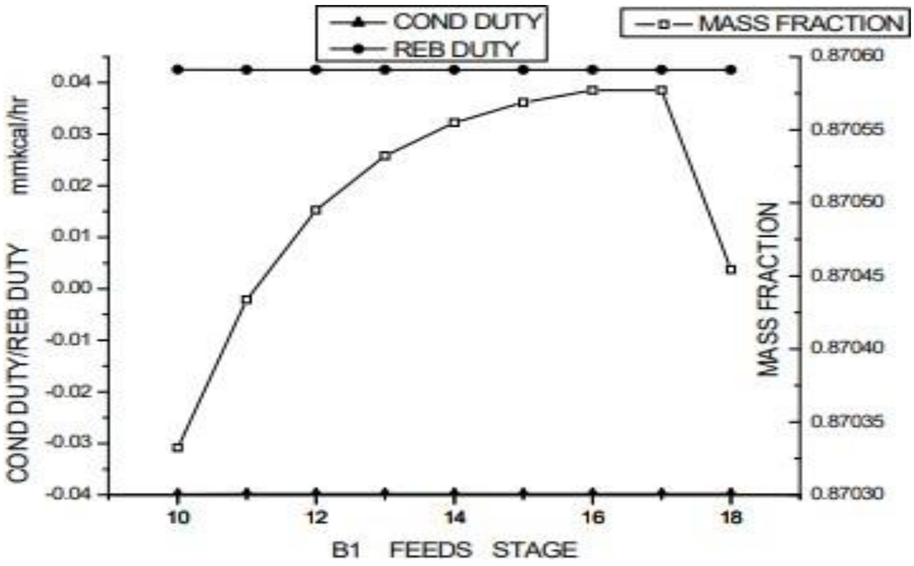

Figure V. The Effect Of Feed Stage On Mass Fraction Of Acetonitrile , Heat Duty Of Reboiler And Condenser In Vacuum Tower.

Establish an Optimization Model According to the features of pressure-swing distillation system, the optimization model of minimal energy consumption of distillation process was established under the premise assuring the quality of products to obtain energy efficient optimizing operation parameters. In which, the stage number of two towers were changeless, and the target function (Minimum total heat duty), constraint condition, control variables wereas follows:

Target function: Y= min (B1REB-B1COND+B2REB-B2COND) Constraint condition: w(CH3CN)≥0.999 Control variables:

1) Vacuum tower: R: 0.1≤R≤3.0; NF: 14≤NF≤17;
P(bar): 0.0≤P≤0.4;
D(kg•h-1): 50≤D≤60

2) Pressurized tower:R: 0.1≤R ≤3.0; NF: 12≤NF≤16; P(bar): 3.0≤P≤4.0

Results :

Results of optimization were as follows:
In vacuum tower: R=2.0, P=0.4bar, NF=16, D=57kg/hr; in pressurized tower: the R=0.58, P=3.5bar, NF=12.

The vacuum system was applied to the Azeotropic distillation column At last, the simulation was carried out again with optimized parameters, the results were obtained as TABLE III. The total heat duty of pressure-swing distillation system was reduced from 0.14634 to 0.10925(mmkcal/hr),increase in purity of desired product as will as saved energy 25%, which showed that the optimization of process parameters reached the expected effect.

TABLE III. THE OPTIMIZED RESULTS OF DISTILLATION TOWERS

Column	The optimize result of column							
	Stream	Tempe-rapture (^{0}C)	Pressure (bar)	Acetonitrile mass fraction	Moisture mass fraction	Massflow	Heat duty	
Vacuum tower	1-RAW-IN	25.0	1.00	0.5000	0.5000	100.00	TOP	-0.03982
	2-GF-OUT	51.5	0.40	0.8706	0.1294	57.432	TOP	-0.03982
	2-WAT-O	75.9	0.40	32PPM	1.000	42.562	KETTEL	0.04249
Pressurized tower	5-GF-IN2	52.1	4.00	0.8706	0.1294	57.432	TOP	-0.01150
	3-REC-O	116.5	3.50	0.7612	0.2388	31.121	TOP	-0.01150
	6-PROD-O	126.6	3.50	1.000	45PPM	26.311	KETTEL	0.01428

CONCLUSION:

1) The vacuum system was applied to the Azeotropic distillation column and NRTL thermodynamics model and Radfrac distillation model were chosen and used to calculate the distillation process, the mass fraction of acetonitrile and water attained the separating demand through the simulation, as the consequence, the established model could be used to simulate the process of pressure-swing distillation.

2) The influence of process parameters such as reflux ratio or feed stage-NF, tower pressure-P and distillate flow rate-D on the rectification effect was analysed by sensitivity analysis tools. The optimization model of minimal energy consumption of distillation process was established under the premise assuring the quality of products, and the energy-efficient optimizing operation parameters were obtained. Ultimately, the results show that increase in quality of product by 5-7% and energy loss decreased 25% by optimized operating parameters in the separation process, which laid the foundation for design and implementation of real-time optimization control system.

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