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# Comparison of pressure-swing distillation and extractive distillation with varied-diameter column in economics and dynamic control



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### ARTICLE INFO

Article history: Received 24 May 2016 Received in revised form 9 November 2016 Accepted 17 November 2016 Available online 28 November 2016

Keywords: Pressure-swing distillation Extractive distillation Varied-diameter column Economics Dynamic control

# ABSTRACT

Pressure-swing distillation and extractive distillation are two common methods for azeotrope separation. The economics and controllability are two crucial factors for evaluating the feasibility of a separation process. A varied-diameter column (VDC) was used in the process design to evaluate its economics and controllability. Five azeotropic systems were investigated in order to compare the economics of pressure-swing distillation and extractive distillation with a VDC. Results indicate that pressure-swing distillation with a VDC saves more money than extractive distillation. The dynamic control were evaluated in the acetone-methanol system for both processes with a VDC. The improved control structure for pressure-swing distillation with a VDC can only handle  $\pm 10\%$  disturbances. A comparison of the two methods from the viewpoint of economics and controllability demonstrates that pressure-swing distillation is more suitable when using a VDC.

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### 1. Introduction

Distillation is the principal separation method in the chemical and petroleum industries. Its importance is well known in chemical industry [1]. Distillation is based on differences in the compositions between the liquid and vapor phases. Mixtures with ideal or near-ideal vapor-liquid equilibrium behavior can be separated by conventional distillation processes [2]. The separation of azeotropes and close-boiling mixtures, however, is a challenging task in many chemical processes. Some special distillation processes, such as azeotropic distillation [3–7], pressure-swing distillation [8–17], and extractive distillation [18–26] have been used to solve this problem.

Pressure-swing distillation is based on the variation in azeotropic compositions under different pressures [27]. Efficient separation is achieved by using two columns operating at two different pressures, which are determined by the composition variation of the azeotrope with pressure. The volatilities of components to be separated are altered by using an additional component for extractive distillation [2]. The azeotrope is separated using two columns: the extractive and solvent recovery columns. Two high-

http://dx.doi.org/10.1016/j.jprocont.2016.11.005 0959-1524/© 2016 Elsevier Ltd. All rights reserved. purity products are obtained at the top of the two columns, and the recovered solvent at the bottom of the solvent recovery column is recycled to the extractive column. To date, many scholars have made comparisons between pressure-swing distillation and extractive distillation from the viewpoint of steady state simulation and dynamic control [28–32]. For example, Luo et al. [29], explored pressure-swing distillation and extractive distillation for separating isopropyl alcohol-diisopropyl ether; the optimal design and dynamic control of the two processes were investigated to make a comparison. Hosgor et al. [32] compared the two processes for separating methanol-chloroform and explored the controllability of pressure-swing distillation on the basis of economic advantages.

Economic analysis is the crucial factor in a steady state comparison. Total annual cost (TAC) [33,34] that includes capital investment and operating cost, is usually considered as the objective function for evaluating the distillation process. To minimize the TAC, many efforts have been devoted to various kinds of heat integrations, such as partial heat integration [35,36] and full heat integration [37], internal heat integration [38] and external heat integration [39,40], and so on.

Dynamic control, which is another important aspect of the distillation process, has also been explored in many papers [41–48]. Both pressure-swing distillation and extractive distillation processes have various control schemes for systems under diverse conditions. For example, Luyben [48] suggested several control schemes

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Notation				
VDC	Varied-diameter column			
TAC	Total annual cost			
PI	Proportional and integral			
HE	Heat exchanger			
CS1	Basic control structure of pressure-swing distilla-			
	tion			
CS2	Improved control structure of pressure-swing dis-			
	tillation			
CS3	Basic control structure of extractive distillation			
CS4	Improved control structure of extractive distillation			
R2/F	Reflux flow rate of the second column/feed flow rate			

of pressure-swing distillation for separating a maximum-boiling azeotropic mixture of methanol and trimethoxysilane. Wang et al. [47] studied the design and control of methylal-methanol separation by extractive distillation; a control structure with the reflux flow rate/feed flow rate ratio scheme was used to maintain the purity requirements of the two products. Wei et al. [45] investigated two control structures for separating dimethyl carbonate-methanol using pressure-swing distillation. All studies on control structure and selection of control variables can promote the application of dynamic control in the chemical processes.

In published studies, researchers studying the pressure-swing distillation and extractive distillation processes adopted a column with equal diameters. However, a varied-diameter column (VDC) has been used in the industry. The diameter of a column is determined by the flow of gas and liquid in the column. A VDC is adopted if the flow of gas and liquid in different sections of the column varies considerably. When it comes to a new system, Tray Sizing feature of Aspen Plus can determine the suitable diameter, and the change in column diameter could be analyzed by plotting the calculated diameters along the stages. Adopting the suitable diameter in different column sections could improve the hydraulics performance, avoid drift during low load operation, and improve the plate efficiency. It is also useful for reducing the capital cost by varying the diameter when the flow of gas and liquid is fairly different between the rectifying and stripping sections. The economics and controllability of pressure-swing distillation and extractive distillation processes adopting a VDC are yet to be discovered.

In this paper, five binary azeotropic systems (acetonechloroform, acetone-methanol, methanol-chloroform, benzenecyclohexane, and isopropyl alcohol-diisopropyl ether) are used as case studies for separation by pressure-swing and extractive distillation. Unlike past simulation, a VDC is adopted to evaluate the pressure-swing and extractive distillation processes, with respect to their economics and controllability, to find which process better suits the distillation.

## Table 1

Results of correlation in five systems with three thermodynamic models.

rate of the second column/leed now rate	azeotropes. In this section, the methanol-chloroform system was
	discussed in detail to illustrate the process simulation procedure
	and economic analysis.

# 2.1. Process simulation

are shown in Table 1.

The basic parameters of the methanol-chloroform system were the same as those in previously published work [32]. The pressure of the two column was 1 and 10 atm, respectively. NRTL physical property package was used in the process. The azeotropic compositions vary from 65.75 mol% methanol (1 atm) to 41.89 mol% methanol (10 atm). The feed flow rate was set as 100 kmol/h, and contained 50 mol% each of methanol and chloroform at 300 K. The products' purity was set to 99.5 mol%. A sequential iterative optimization method [32,55,56] was used to obtain the optimal design parameters on the basis of minimizing TAC (Fig. S1).

2. Steady state simulation and economic analysis

Five azeotropic systems that were studied in previous papers [29,30,32,44,49] were simulated by both pressure-swing and extractive distillations in Aspen Plus. Before simulating, the thermodynamic models of the separating processes were validated. The predicted values using the thermodynamic models fit well with experimental vapor liquid equilibrium data [50–54]. The results

Fig. 1 depicts the Txy curves of the five azeotropic systems. Acetone-chloroform is the maximum-boiling system, while the other four systems are minimum-boiling azeotropes. Results indicate that pressure-swing distillation can be used to separate the five

In order to demonstrate which factors influence the diameter, an procedure for calculating the diameter was explored. The relevant parameters were obtained from a simulation using Aspen Plus.

The common procedure for calculating the diameter of a column is illustrated by Eq. (1):

$$D = \sqrt{\frac{4V_S}{\pi u}}$$
(1)

where D indicates the column diameter, m;  $V_S$  is the column gas flow,  $m^3/s$ ; and u is the gas velocity of an empty column, m/s.

The gas velocity of an empty column is determined by the maximum allowable gas velocity,  $u_{max}$ , which can be calculated according to Eq. (2):

$$u_{max} = C \sqrt{\frac{\rho_L - \rho_V}{\rho_V}}$$
(2)

where  $\rho_L$  is the liquid phase density, kg/m<sup>3</sup>;  $\rho_V$  is the vapor phase density, kg/m<sup>3</sup>; and C is the load coefficient, m/s.

The load coefficient (C) is determined from the Smith Correlative Graph [57].

With the aid of a Smith Correlative Graph, the load coefficient with surface tension of liquid ( $\sigma$ ) = 20 mN/m (C<sub>20</sub>) is obtained.

C is calculated according to Eq. (3):

$$C = C_{20} \left(\frac{\sigma}{20}\right)^{0.2} \tag{3}$$

Azeotropic system	Selected model	Residual root mean square error		
		UNIQUAC	NRTL	WILSON
Acetone-chloroform	UNIQUAC	1.841	2.278	2.429
Acetone-methanol	UNIQUAC	0.888	0.903	0.0972
Methanol-chloroform	NRTL	1.443	1.412	3.022
Benzene-cyclohexane	NRTL	1.045	1.011	1.110
Isopropyl alcohol- diisopropyl ether	NRTL	2.776	2.630	3.120

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