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Comparative Analysis: Trays versus Packed Columns in Pressure-Swing Distillation for the Separation of Tetrahydrofuran, Water and Ethanol Azeotropic Mixture

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Abstract

This paper delves into the comparative study of tray and packed column pressure swing distillation systems, focusing on the separation of a ternary mixture containing ethanol, tetrahydrofuran (THF), and water. The study particularly emphasizes the production of 99.5 w/w% tetrahydrofuran from the downstream product of 1,4-butanediol synthesis via diethyl maleate. Pro/II simulation software is utilized to explore various system configurations, including sieve trays, valve trays, and packed columns. Material and energy balances are performed to ascertain stream compositions and energy demands. The investigation encompasses the effects of column operating pressure on condenser and reboiler temperatures, as well as the implications of utility streams. A rigorous distillation model is employed to compare valve tray, sieve tray, and random packing (utilizing Norton Super Intalox) column designs by varying the number of trays, reflux ratio, and second distillation column pressure. Heat exchangers are integrated into the model, and their areas and utility flow rates are computed and integrated into the economic assessment. Economic analysis, guided by Net Present Value (NPV) calculations over a 20-year span, drives the selection of the most cost-effective design. Results demonstrate that while all designs are energy-efficient, the packed column system emerges as the most economical choice, offering a comprehensive framework for the separation process. Furthermore, optimal design configurations and operating conditions for both tray and packed column systems are outlined, providing valuable insights for industrial applications.

Keywords

Azetrope, Tetrahydrofuran, Ethanol, Pressure-Swing, Distillation, Simulation

1. Introduction

The separation of chemical mixtures is a fundamental process in various industries, crucial for ensuring product purity and meeting regulatory standards. Just as the human body relies on the kidney to separate waste from water for proper metabolism, industrial processes require efficient separation mechanisms to remove impurities and isolate desired components. Distillation stands as a cornerstone method for achieving such separations, yet its efficacy can be challenged when faced with azeotropic mixtures—complex combinations where traditional distillation falls short [1] [2]. One such intricate scenario arises in the production of 1,4-butanediol from maleic anhydride, yielding a ternary azeotropic mixture comprising ethanol, tetrahydrofuran (THF), and water. Achieving the desired purity of products within this mixture presents a formidable challenge to conventional distillation methods. However, advancements in distillation technology such as pervaporation membrane [3] [4], extractive distillation [5], azeotropic distillation [6], pressure swing distillation [7]-[11], and offer promising solutions, with pressure swing distillation emerging as a leading contender for its simplicity and effectiveness [12]. Pressure swing distillation, a technique that manipulates column pressure to facilitate separation, has garnered attention for its ability to address azeotropic challenges without introducing additional substances or requiring adsorbents. Its streamlined approach and potential for high-purity product streams make it an attractive option for industries striving for efficiency and compliance. In this paper, we delve into the comparative study of tray and packed columns pressure swing distillation systems tailored for the separation of the ethanol, THF, and water azeotropic mixture encountered in the production of 1,4-butanediol. Our investigation, conducted through Pro/II simulation software, meticulously examines various column configurations and operational parameters to identify optimal design configurations. Beyond exploring technical aspects, we conducted economic analyses to evaluate the cost-effectiveness of each design, guided by Net Present Value (NPV) considerations over a twenty-year timeframe. By elucidating both technical and economic dimensions, this study aims to provide comprehensive insights into the design and optimization of pressure swing distillation systems, offering practical guidance for industrial applications seeking efficient separation solutions amidst complex chemical mixtures.

2. Thermodynamics of Ethanol (EtOH) C_2H_5OH, Tetrahydrofuran (THF) and Water (H_2O) Mixture

Ethanol, Tetrahydrofuran (THF) and water mixture is a ternary mixture with the ternary diagram shown in **Figure 1**. The residual curve shown in **Figure 1** is

tangent to the vapour-liquid equilibrium tie line that cannot be crossed. However, due to the parabolic shape at the top of the residual curve, it is possible to achieve the necessary separation, despite the azeotropic nature of water, tetrahydrofuran and ethanol [5].

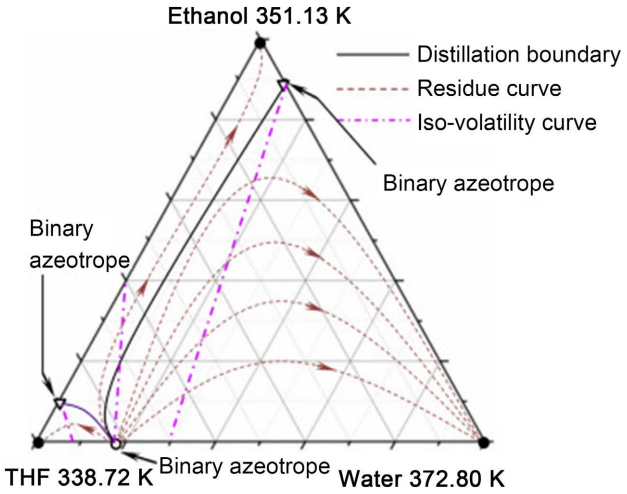

Figure 1. Triangular diagram for THF-EtOH and H_2O mixture.

THF and water forms a binary mixture with an azeotropic composition of 95 w/w% of THF at atmospheric pressure [13]. The properties of azeotropic mixture can be described using Dalton law and modify Raoults law [14]. For a tetrahydrofuran and water binary mixture, the partial pressure of tetrahydrofuran (P_{THF}) can be expressed as:

$$P_{THF} = y_{THF} P_T \tag{1}$$

where y_{THF} is THF vapour mole fraction and P_T is the total pressure.

The modified Raoult's law expression for tetrahydrofuran and water binary mixture can be expressed in terms of the tetrahydrofuran vapour pressure p_{THF}^{vap}, mole fraction in liquid phase (x_{THF}) and the activity coefficient (γ_{THF}) as:

$$P_{THF} = x_{THF} p_{THF}^{vap} \gamma_{THF} = y_{THF} P_T \tag{2}$$

It can be seen from Equation (2) that the azeotropic composition changes with pressure. This variation is illustrated in the T-x-y and x-y diagrams shown in **Figure 2** and **Figure 3** respectively.

The T-x-y and x-y diagrams of THF-water mixture were generated by Pro/II respectively, and both figures show that the azeotropic composition of THF changes from about 0.83 mol% at atmospheric pressure to about 0.68 mol% at a pressure of 7.6 bar.

3. Material and Energy Balance

3.1. Overall Material Balance

An overall material balance was performed on the proposed pressure swing dis-

tillation system for the separation of THF from water-THF-EtOH azetropic mixture (Figure 4) using Equation (3) to obtain the streams' compositions shown in Table 1.

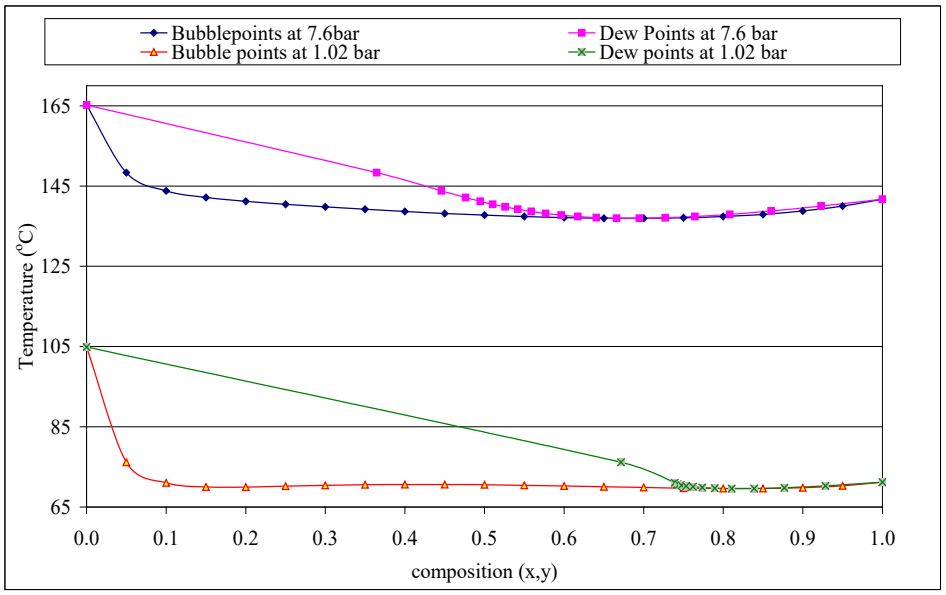

Figure 2. T-x-y of THF-H_2O mixture.

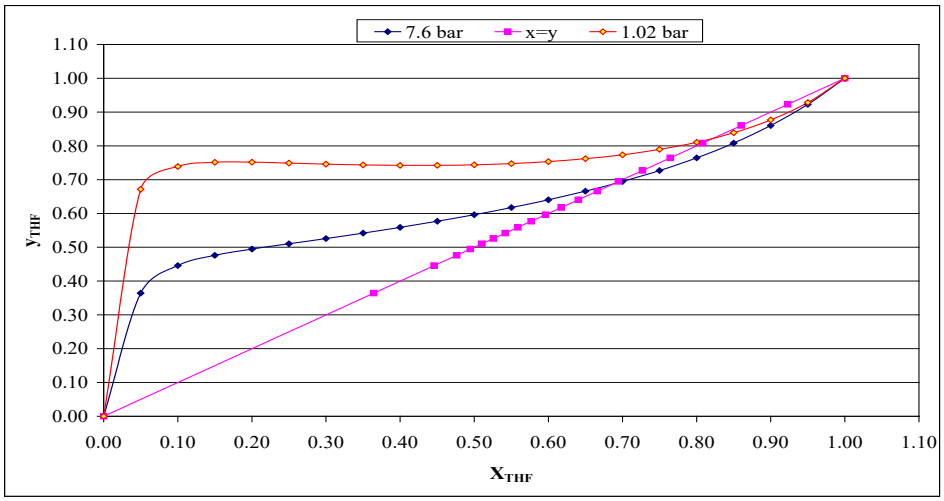

Figure 3. x-y diagram of THF-water mixture at a pressure of 1.02 bar and 7.6 bar.

$$\text{Input} - \text{Output} + \text{Generation} - \text{Dissipation} = \text{Accumulation} \quad (3)$$

where T1 and T2 represent the two distillation columns operated at 1.02 and 7.6 bar, and S represents the stream.

Streams S4 and S5 were obtained by performing an overall material balance for THF, EtOH, H_2O and BuOH.

The following assumptions were made:

- Inlet stream flow rate (5.12 kmol/hr THF, 5.28 kmol/hr H_2O, 164.47 kmol/hr Ethanol (EtOH) and 0.17 kmol/hr Butanol (BuOH)).

- Azeotropic overhead product composition of both columns.
- No reaction occurs and therefore, there is no generation nor dissipation.
- Steady state and therefore there is no accumulation.
- All light components are completely separated from the heavy components.

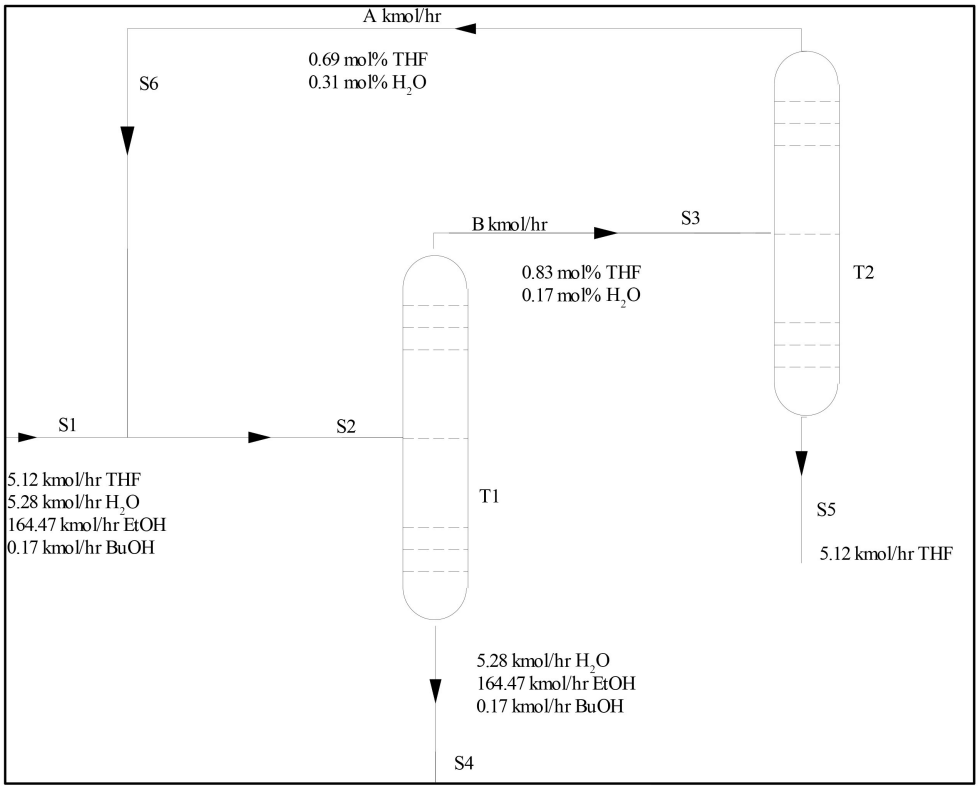

Figure 4. Pressure swing distillation system flow diagram.

Table 1. Material balance of the pressure swing separation system.

Stream	Component	Molar Flow rate (kmol·hr^{-1})	Composition	Phase
S1	THF	5.120	0.029	Liquid
	H_2O	5.280	0.030	Liquid
	EtOH	164.470	0.940	Liquid
	BUOH	0.170	0.001	Liquid
	Total	175.040	1.000	Liquid
S2 (T1 Input)	THF	9.410	0.052	Liquid
	H_2O	7.207	0.040	Liquid
	EtOH	164.470	0.907	Liquid
	BuOH	0.170	0.001	Liquid
	Total	181.257	1.000	Liquid
S3 (T1 Distillate)	THF	9.410	0.830	Liquid
	H_2O	1.927	0.170	Liquid
	Total	11.337	1.000	Liquid

Continued

S4	EtOH	164.470	0.968	Liquid
	H_2O	5.280	0.031	Liquid
	BUOH	0.170	0.001	Liquid
	Total	169.920	1.000	Liquid
S5	THF	5.120	1.000	Liquid
S6	THF	4.290	0.690	Liquid
	H_2O	1.927	0.310	Liquid
	Total	6.217	1.000	Liquid

3.2. Overall Material Balance

An energy balance was carried out in order to determine the energy requirements for the condensers and reboilers of the separating system as shown in Figure 5 (Where V, L and D are the vapour flow rate, liquid flow rate and the Distillate). Prior to the energy balance analysis, a material balance was carried out using a reflux ratio of 3 to obtain the flow rate of the various streams and the utilities shown in Tables 2-4. The heat duty of the condensers was calculated using Equations (4) and (5), while the heat duty of the reboilers was calculated using Equations (4) and (6). The results obtained are tabulated in Table 5.

$$\text{Duty}\left(\text{kJ/hr}\right) = \text{Latent heat}\left(\text{kJ/kmol}\right) \times \text{Flow rate}\left(\text{kmol/hr}\right) \tag{4}$$

$$\text{Condenser Heat Duty}\left(Q_c\left(\text{kJ/hr}\right)\right) = \sum_{i=1}^{n} Q_{ci} = \sum_{i=1}^{n} V_i h_{vi} \tag{5}$$

$$\text{Reboiler Heat Duty}\left(Q_R\left(\text{kJ/hr}\right)\right) = \sum_{i=1}^{n} Q_{Ri} = \sum_{i=1}^{n} \left(D\left(R+1\right)\right) h_{vi} \tag{6}$$

where h is the enthalpy and R is the reflux ratio (which was set to a value of 3).

$$V_n = L_n + D \tag{7}$$

$$L_n = RD \tag{8}$$

$$V_n = D\left(R+1\right) \tag{9}$$

$$L_b = V_b = V_m = V_n = D\left(R+1\right) \tag{10}$$

Table 2. Overhead and bottom product of the first distillation column T_1.

Distillation column distillate (Liquid phase)			Distillation column bottom product (Liquid phase)		
Component	Molar Flow rate ($kmol \cdot hr^{-1}$)	Composition	Component	Molar Flow rate ($kmol \cdot hr^{-1}$)	Composition
THF	9.410	0.830	THF	0.000	0.000
H_2O	1.927	0.170	H_2O	5.280	0.031
EtOH	0.000	0.000	EtOH	164.470	0.968
BUOH	0.000	0.000	BUOH	0.170	0.001
Total	11.337	1.000	Total	169.920	1.000

Table 3. Flow rate of the condenser input and T_1 first tray feed.

L_n			Condenser Input (V_n)		
Component	Molar Flow rate (kmol·hr^{-1})	Composition	Component	Molar Flow rate (kmol·hr^{-1})	Composition
THF	28.229	0.830	THF	37.639	0.830
H_2O	5.782	0.170	H_2O	7.709	0.170
EtOH	0.000	0.000	EtOH	0.000	0.000
BUOH	0.000	0.000	BUOH	0.000	0.000
Total	34.011	1.000	Total	45.349	1.000

Table 4. Flow rate of the reboiler input and bottom product of T_1 last tray.

L_m			Reboiler Input (liquid phase)		
Component	Molar Flow rate (kmol·hr^{-1})	Composition	Component	Molar Flow rate (kmol·hr^{-1})	Composition
THF	37.639	0.175	THF	37.639	0.830
H_2O	12.989	0.060	H_2O	7.709	0.170
EtOH	164.470	0.764	EtOH	0.000	0.000
BUOH	0.170	0.001	BUOH	0.000	0.000
Total	215.269	1.000	Total	45.349	1.000

Table 5. Condenser and reboiler heat duties.

Component	Latent Heat		Heat duty (kJ·hr^{-1})	
	kJ·kg^{-1}	kJ·kmol^{-1}	Condenser	Reboiler
THF	410.00	29520.00	−1111112.56	1111112.56
H_2O	2261.11	40700.00	−313766.77	313766.77
EtOH	480.49	39400.00	0.00	0.00
BUOH	920.00	68080.00	0.00	0.00
Total	–	–	−1424879.32	1424879.32

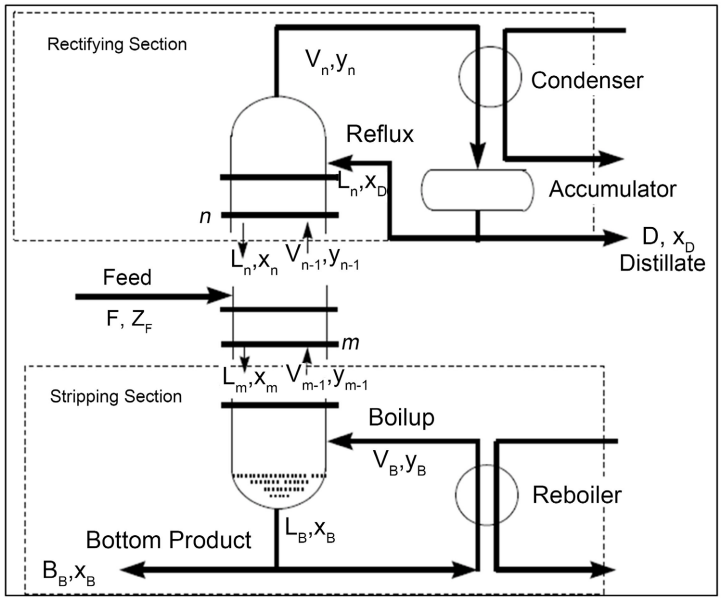

Figure 5. Geometry of a distillation column.

4. Simulation Design & Optimisation Swing System

4.1. Introduction

The design of the pressure swing distillation system was carried out using Pro/II. Sieve trays, valve trays and packed distillation columns were investigated due to their merits [15]. For the trays columns (*i.e.* sieve and valve trays), tray's efficiency, minimum reflux ratio, optimum number of trays, feed location, and optimum pressure for the second column were investigated as described by Towler and Sinnott [1]; while for the packed columns, in addition to the minimum reflux ratio, and second column optimum pressure investigated, the optimum packing height and equivalent feed tray location were also investigated as described by Towler and Sinnott [1].

4.2. Design and Optimisation of Trays (Sieve and Valve) Distillation Columns

4.2.1. Geometry Configuration of Trays Columns

Trays with an internal hole diameter of 0.381 m and a tray spacing of 0.609 m were chosen and used for the design of the sieve and valve tray columns.

4.2.2. Trays Efficiency

The tray efficiency of the sieve and valve trays was calculated from the composition results generated by Pro/II, using the Mupheree tray efficiency equation below:

$$\eta_m = \frac{y'_n - y'_{n-1}}{y^*_n - y'_{n-1}} \tag{11}$$

where y'_n = actual vapour composition leaving plate n;

y'_{n-1} = actual vapour composition entering plate n;

y^*_n = Vapour composition in equilibrium with liquid leaving plate n.

The results obtained are tabulated and shown in Table 6.

Table 6. Mupheree tray efficiency for sieve and valve trays.

Tray types	Mupheree Efficiency
Sieve	0.816
Valve	0.814

4.2.3. Trays Efficiency

The minimum reflux ratio of both distillation columns was investigated columns as the simulation software cannot operate if either column is operated below this threshold. To achieve this, the number of trays in each column was incrementally increased until the reflux ratio stabilized. The results obtained from PRO/II for both columns, utilizing sieve and valve trays respectively, are depicted in Figure 6 and Figure 7. As illustrated in Figure 6, with an increase in the number of trays, the reflux ratio steadily decreases until it reaches its minimum value. Beyond this point, further additions of trays have no significant impact on the

reflux ratio. This observation aligns with findings in the literature [16] [17]. Additionally, Figure 6 reveals that the minimum reflux ratio for column T1 is 46.50, whereas for column T2, it is 2.20. The higher reflux ratio in column T1 is attributed to the elevated ethanol content in the mixture. Figure 7 highlights that the minimum reflux ratio for column T1, using valve trays, is 50, while for column T2, it remains consistent with that obtained for the sieve trays. Discrepancies in the minimum reflux ratio for column T1 could stem from differences in tray geometry configurations.

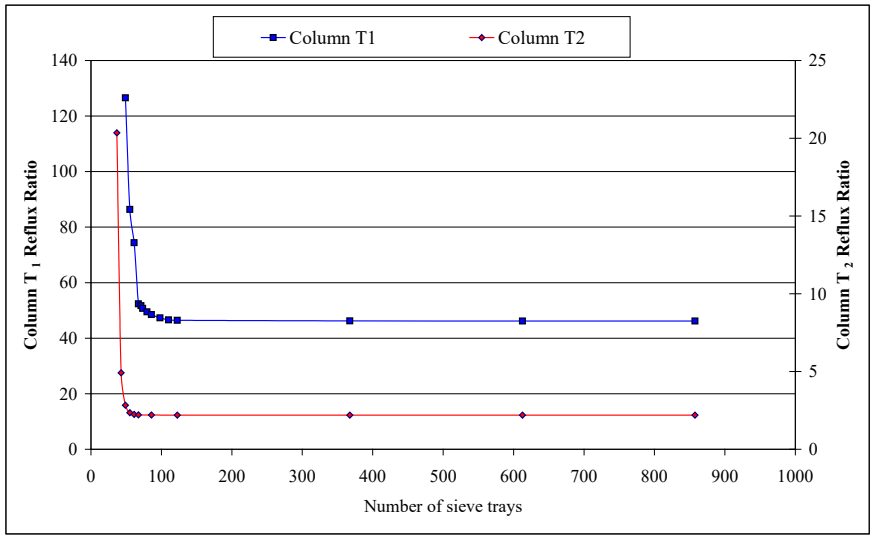

Figure 6. Investigation of the minimum reflux ratios of both columns using sieve trays.

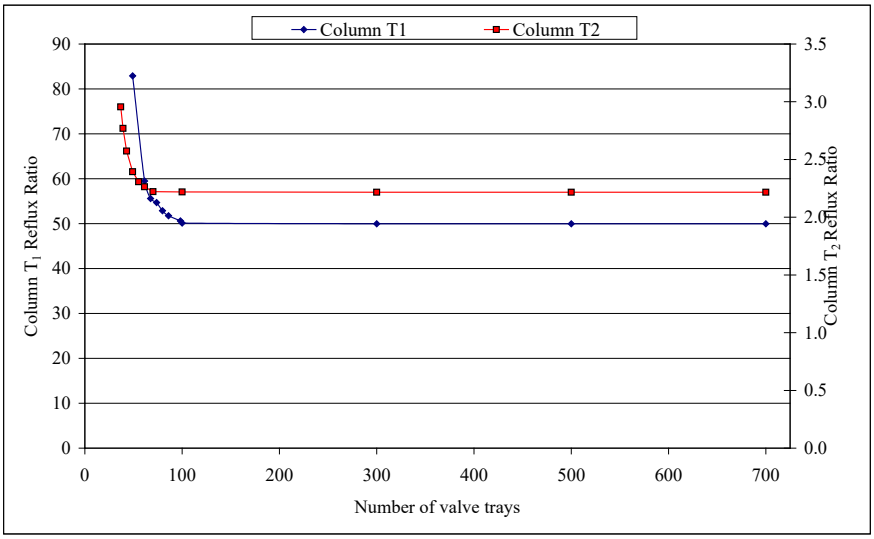

Figure 7. Investigation of the minimum reflux ratios of both columns using valve trays.

4.2.4. Investigation of the Optimum Number of Trays

For the sieve trays distillation columns, the first distillation column (T1) number of trays was optimized first by changing the number of trays while all other variables were kept constant, including the number of trays of the second column

(T2). Each time the number of trays was changed, the software was run and the Net Present Value for a period of twenty years was calculated using the results generated by PRO/II. The capital cost of the heat exchangers, column shells and trays were calculated. After which, the total capital cost, operating cost, and the net present value (NPV) were calculated. The configuration that yielded the lowest NPV value was chosen as the optimum number of trays for the first column. The optimum number of trays for the first column was used to optimise the second tray, whereby only the second column number of trays was varied. The NPV of the second column was also calculated. The results obtained are shown in Figure 8. The same method was used for valve trays distillation columns and the results obtained are shown in Figure 9.

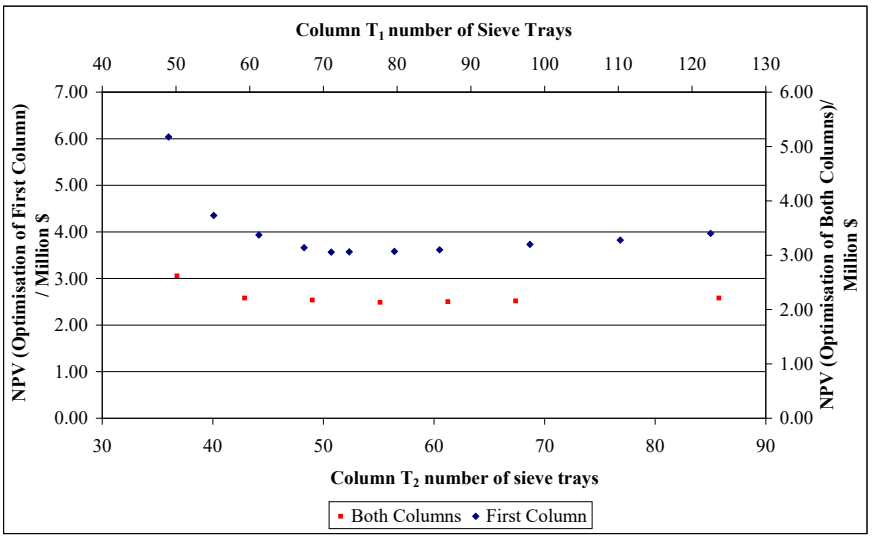

Figure 8. Optimisation of the number of trays of the sieve trays pressure swing distillation columns.

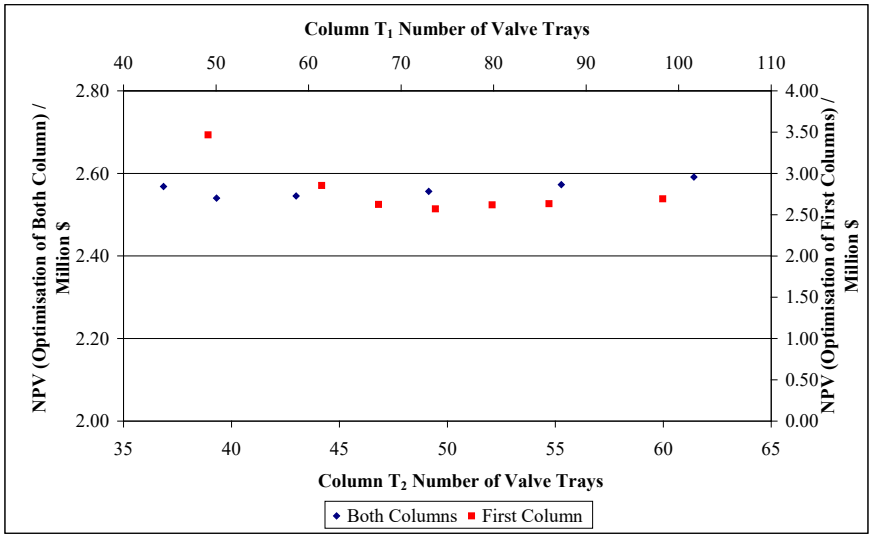

Figure 9. Optimization of the number of trays in the valve trays pressure-swing distillation columns.

Figure 8 shows that the optimum number of sieve trays for column T1 and column T2 are 71 and 55 trays respectively as they incurred the lowest net present. The NPV decreases initially before increasing, as the number of trays increases. This is because initially, at low number of trays, the reflux ratio was high leading to high utilities and therefore high operating cost, which made the operating cost the controlling factor of the total cost. However, as the number of trays increases, the separation also increases which leads to the smaller amount of reflux and heat duties required by the reboilers and condensers. The decrease of NPV with an increasing number of plates continued until the minimum cost was achieved. The further increase in the number of trays will cause an increase in the NPV value due to capital cost, thus making the capital cost the controlling factor. It can be deduced from Figure 9 that the optimum number of valve trays for column T1 and column T2 are 74 and 39 trays respectively, as they yield the lowest net present value (NPV). This is however higher than the NPV obtained for the optimum sieve trays.

4.2.5. Investigation of Second Column (T2) Optimum Pressure

Research conducted by Iqbal and Ahmad [8], Liang *et al.* [9], and Wang *et al.* [10], highlighted the optimal operating conditions for pressure swing distillation systems. According to the literature, the first column of the system should operate at atmospheric pressure, while the second column's pressure is ideally maintained within the range of 5 - 10 bar. Consequently, our investigation focused solely on the pressure of the second distillation column, exploring values within the recommended range (5 - 10 bar). For each pressure value investigated, the Net Present Value (NPV) was calculated and plotted, as depicted in Figure 10 and Figure 11 for sieve and valve tray columns respectively. These figures provide insights into the economic implications of varying the pressure within the specified range, aiding in the selection of the most cost-effective operating conditions for the distillation system.

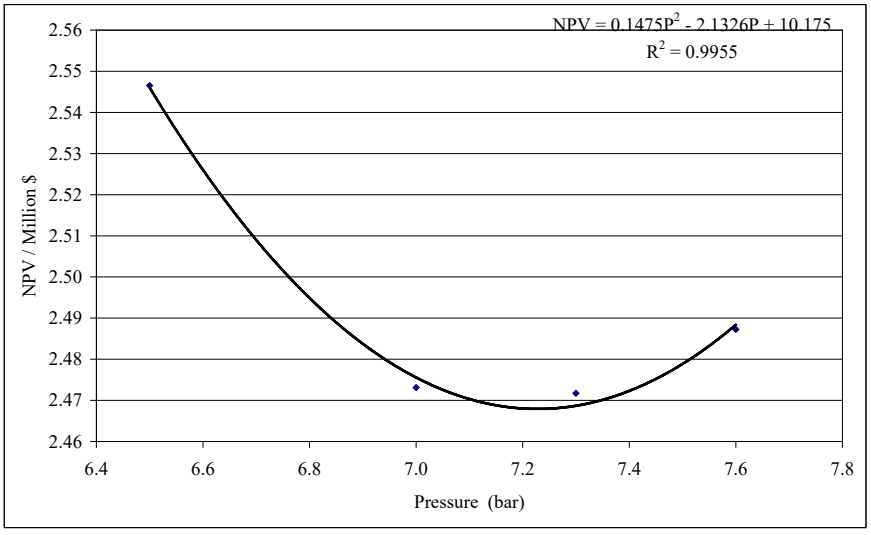

Figure 10. Sieve tray distillation column T2 optimum pressure.

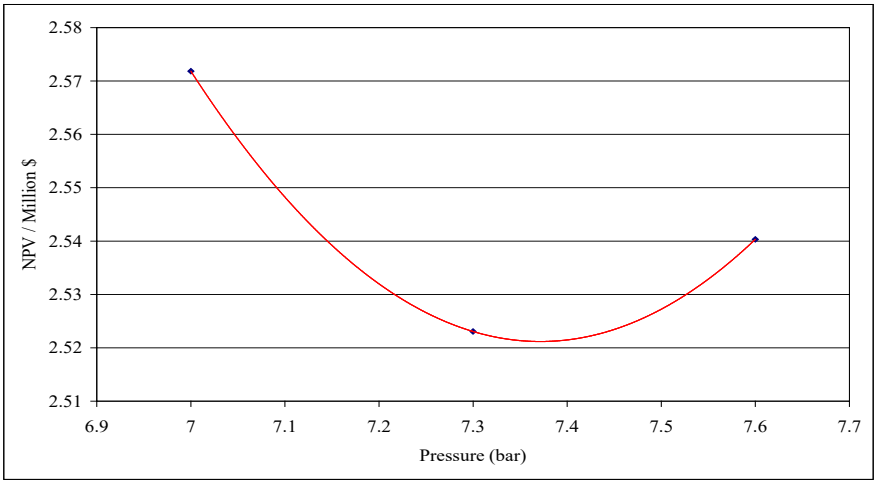

Figure 11. Valve trays distillation Column T2 optimum pressure.

Figure 10 illustrates that the optimal operating pressure for the second distillation column equipped with sieve trays is 7.2 bar, while **Figure 11** demonstrates that for the valve tray column, it is 7.4 bar. Both figures indicate that column T2 should be operated within the range of 6.5 - 7.6 bar to ensure feasible separation, as operating outside this range would result in impractical heat exchanger area requirements calculated by PRO/I.

4.2.6. Investigation of Second Column (T2) Optimum Pressure

The optimal feed tray location for both distillation columns was investigated using the optimizer in PRO/II. This investigation aimed to minimize the heat duties of the respective distillation column reboilers and condensers by adjusting the feed tray location for both columns.

4.3. Design and Optimisation of Packed Columns

4.3.1. Geometry Configuration of Packed Columns

The primary function of a packed column is to facilitate intimate contact between gaseous and liquid streams to enhance mass transfer efficiency. This is achieved by allowing the vapor to interact continuously with the downward-flowing liquid over the packing material's length. For this study, a 0.254 m internal diameter of super Intalox saddles random packing, manufactured by Norton, with a packing factor of 196.85 $m^2 \cdot m^{-3}$, was employed.

4.3.2. Investigation of the Minimum Reflux Ratio of Both Columns

This was carried out by increasing the packing height of each column continuously until the reflux ratio became constant. It can be seen from **Figure 12**, that the minimum reflux ratio for column T1 and T2 are 44.50 and 2.15 respectively.

4.3.3. Investigation of the Optimum Height of the Packing Material

The optimum packing height was investigated by changing the packing height which in turn, changed the packing volume. The volume of packing material was

calculated, and the cost analysis was performed. The results obtained are shown in Figure 13.

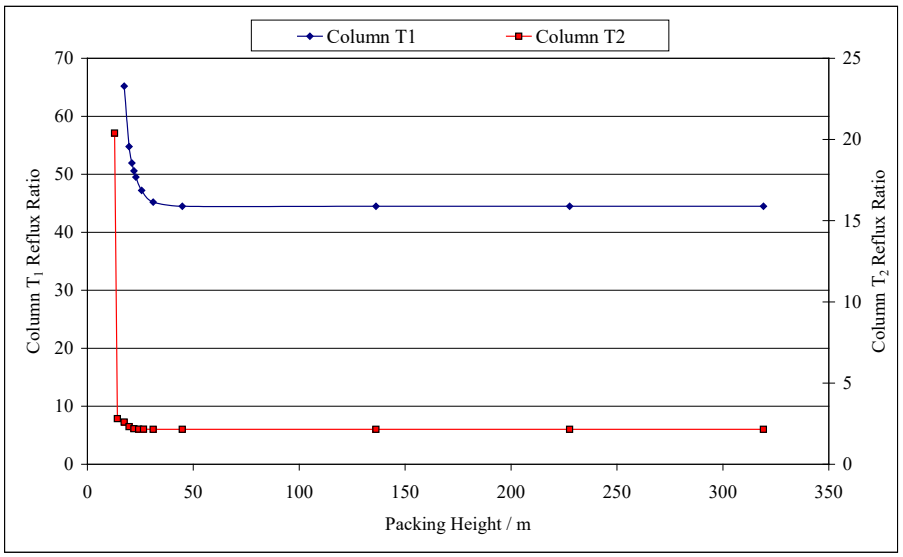

Figure 12. Investigation of the minimum reflux ratios of both columns using Super Intalox saddles as the packing material.

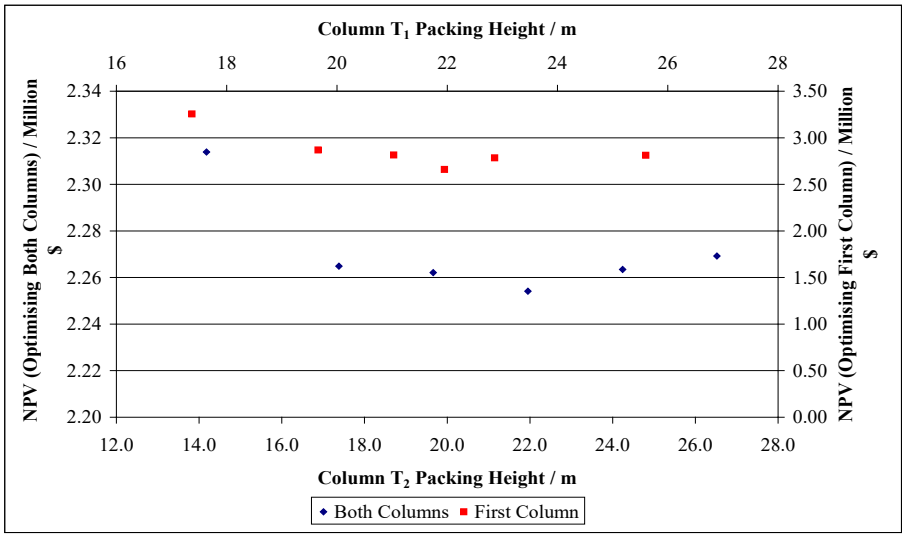

Figure 13. Optimisation of the packing height of distillation column T1.

The optimum reflux ratio is the reflux ratio calculated by PRO/II for the optimum packing height. From Figure 13, the optimum packing height for column T1 and column T2 are both 21.95 m as they yield the lowest net present value.

4.3.4. Investigation of the Second Column (T2) Optimum Pressure

Column T2 pressure was investigated using the same method as that of trays column. The results obtained are shown in Figure 14.

Figure 14 shows that the pressure of column T2 for the packed column has little effect on the net present value. This might be a result of the range of pres-

sure investigated. However, the stimulation software used shows that the separation will be infeasible outside this range. This leads to the conclusion that the optimum pressure for packed column T2 range from 7 bar to 7.8 bar.

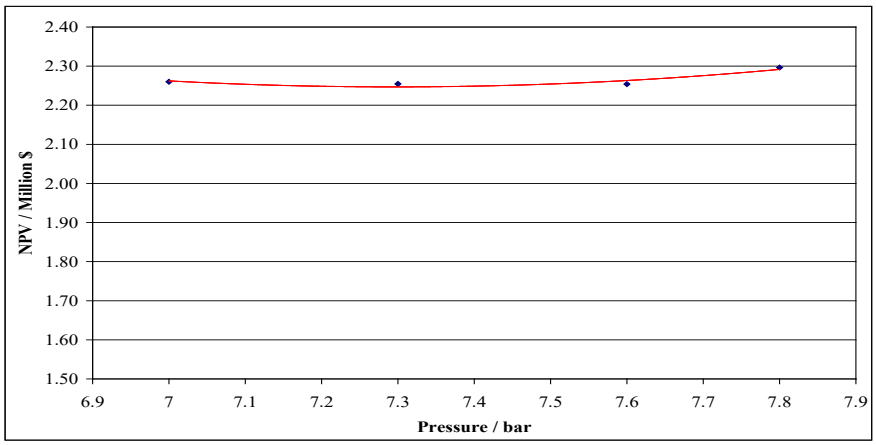

Figure 14. Investigating the optimum pressure of packed distillation Column T2.

4.3.5. Investigation of Distillation Columns' Equivalent Feed Tray Location

The optimum equivalent feed tray location of both columns was investigated using the optimiser in PRO/II to minimise the heat duties of the columns' reboilers and condensers by changing the location of the feed tray of both columns.

5. Economics and Cost Analysis

The most economical operating conditions for the separating system are those that yield the lowest total cost. The cost of electricity, transportation of material, feed or sales of products were not considered in the NPV calculation. It was assumed that the plant will be operated for 20 years after it has been built; the building year is taken as year 0 and the operating hours per annum is 8000 at a discount rate of 0.2. The methodology described by Sinnott *et al.* [7] was used for the cost analysis, including the cost of the various equipment.

5.1. Total Cost of Investment

The total cost of investment includes both the capital and operating costs over a 20-year duration with a discount rate of 0.2. It was calculated using the Equation (12):

$$\begin{aligned}\text{Total Cost} &= \text{Total Capital Cost} + \text{NPV}(20\text{ years}) \\ &= \text{Total Capital Cost} + \left[C_1 + \frac{C_2}{1+d} + \frac{C_3}{(1+d)^2} + \cdots + \frac{C_{20}}{(1+d)^{19}}\right]\end{aligned} \quad (12)$$

where C_n is the operating cost for year n, and d is the discount rate. The cost of feedstock was not incorporated into the equation as this will be constant.

5.2. Total Capital Cost

The total capital cost (C_{TC}) was calculated by summing the cost of the heat exchangers, distillation column shells and packing material as shown in Equation (13).

$$C_{TC} = \sum_{i=1}^{n} C_{HE_i} + \sum_{i=1}^{n} C_{CS_i} + \sum_{i=1}^{n} C_{CM_i} \tag{13}$$

5.2.1. Heat Exchanger Cost

The cost of a heat exchanger (C_{HE}) was calculated using the correlation:

$$C_{HE} = 450\left(\frac{C_1}{315}\right) A_{HX}^{0.7}\left(1.65 + 1.22F_M\left(1 + |P-1|\right)^{0.09}\right) \tag{14}$$

where A_{HX} is the heat exchanger area (between 100 m^2 and 1000 m^2), P is the operating pressure (in barg), C_1 is the cost index and has a value of 500 (from the Chemical Engineering cost index, estimated for the year 2020) and F_M is the material factor. A F_M value of 4 was used as stainless steel was chosen to be used to minimise fouling and corrosion of the heat exchanger.

5.2.2. Column Shell Cost

The cost of the distillation column shell was calculated using the expression:

$$C_{CS} = \frac{C_1}{315}\left(1780L^{0.87}D^{1.23}\right)\left(2.86 + 1.604F_M\left(1.09727 + \left(0.05049 \times |P-1|\right) - \left(-6.82 \times 10^{-5}\left(P-1\right)^2\right)\right)\right) \tag{15}$$

For sieve and valve trays:

$$L = 0.6 \times \left(N_{act} - 1\right) + 5 \tag{16}$$

For packed column:

$$L = h + 5 \tag{17}$$

where h is the height of the packing material and N_{act} is the actual number of trays required, and was calculated as shown below:

$$N_{act} = \frac{N_{\text{theoretical}}}{E_0} \quad \text{(Rounded to the nearest integer)} \tag{18}$$

where D is the column diameter (m), E_0 is the tray efficiency, L is the column height (m), which was calculated using Equations (16) and (17).

5.2.3. Packing Material Cost

For the tray distillation column, the cost of trays was calculated using Equation (19):

$$C_{BM} = \frac{C_1}{315}\left(193.04 + 22.72D + 60.38D^2\right)F_M N_{act} \tag{19}$$

Stainless steel (F_M of 4) was used for the heat exchangers, while carbon steel (F_M of 1) was used for the column shells and trays. This is because steam and

cooling water will be used in the heat exchangers, so therefore, the use of carbon steel will lead to high rate of corrosion, which will in turn contaminate the streams and, eventually reduce the efficiency of the reboilers and condensers.

For packed column, the costs of the various packing material sizes for the Norton Super Intalox saddles are shown in Table 7.

Table 7. Costs of packing material sizes.

Size, mm	$/m^3
25	1000
50	600
75	400

The packing volume was calculated using Equation (20):

$$V_{act} = \frac{V_{\text{calculated}}}{0.8} = \frac{\pi \frac{d^2}{4} h}{0.8} \tag{20}$$

where V_{act} is the actual volume required, and $V_{\text{calculated}}$ was calculated using the dimensions obtained from Pro/II. The column was designed to ensure that the height was not above 60 m.

5.3. Utility Operating Costs

The utility operating cost was deduced as the sum of all the costs of the utilities used (*i.e.* costs of steam and cooling water). This was calculated based on the utility specification as shown in Table 8.

Table 8. Utility specifications.

Utility	Cooling water	Steam
Available at, (K)	303	–
Maximum discharge temperature, (K)	313	–
Saturation pressure (barg)	Supply: 4; Return: 1.2	3.5
Cost	$0.20/m^3	$4/tonne

6. Comparative Analysis

The cost analysis of the three designed THF-H_2O-EtOH azeotropic mixture separating systems was used to perform the comparative study. As shown in Figure 15, the most efficient pressure swing system design based on the cost analysis is the packed column as it generates the lowest NPV value of $2.25 million for a period of twenty years. The sieve and the valve columns generate NPV value of $2.47 million and $2.52 million respectively. However, all three designs are energy efficient and the difference in cost is not copious; thus, any of these three designs can be used for the separation of ethanol, tetrahydrofuran, and water system.

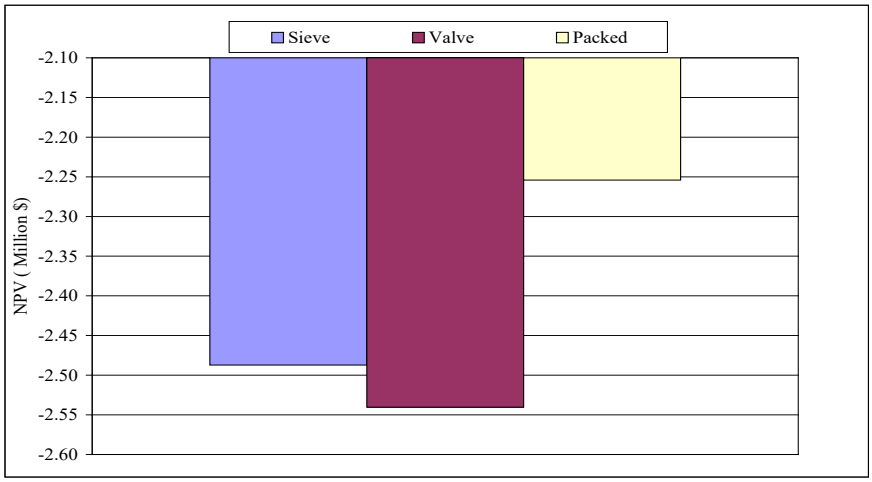

Figure 15. Pressure swing system cost analysis.

The recommended optimum design configurations for the packed column pressure swing system are the following: (**Tables 9-11**)

Table 9. Design configuration of packed pressure swing distillation columns.

Column	Design Configuration	
First column, T_1	Column Shell material: Carbon Steel	Pressure: 1.02 bar
	Packing Height: 21.95 m	Column height: 26.95 m
	Column Internal diameter: 2.60 m	Packing Diameter: 254 mm
	Fresh feed Tray location: 27	Reflux Ratio: 51.59
	Recycle tray location: 27	
Second column, T_2	Column Shell material: Carbon Steel	Pressure: 7.3 bar
	Packing Height: 21.95 m	Column height: 26.95 m
	Column Internal diameter: 0.40 m	Packing Diameter: 254 mm.
	Fresh feed Tray location: 19	Reflux Ratio: 2.19

Table 10. Design configuration of packed pressure swing distillation columns' heat exchangers.

Function	Heat Exchanger			
	E_1	E_2	E_3	E_4
	Condenser	Reboiler	Condenser	Reboiler
Type	Horizontal shell side	Horizontal thermosyphon	Horizontal shell side	Horizontal thermosyphon
Area (m^2)	193	100	100	100
Overall heat transfer coefficient	0.8	0.8	0.8	0.8
FT factor	0.8	0.8	0.8	0.8
Material	Stainless steel	Stainless steel	Stainless steel	Stainless steel

Table 11. Utility specification for packed pressure swing distillation columns' heat exchangers.

Heat Exchanger	Utility				
	Utility Type	Mass flow rate ($te \cdot hr^{-1}$)	Pressure (barg)	Temperature in (K)	Temperature out (K)
E_1	Cooling water	390.25	4	303	313
E_2	Steam	4.61	3.5	421	–
E_3	Cooling water	22.77	4	303	313
E_4	Steam	0.27	3.5	421	–

The recommended optimum design configurations for the sieve trays column pressure swing system are as follows: (Tables 12-14)

Table 12. Design configuration of sieve tray pressure swing distillation columns.

Column	Design Configuration	
First column, T_1	Column Shell material: Carbon Steel	Pressure: 1.02 bar
	Number of trays: 71	Column height: 47.04 m
	Column Internal diameter: 1.83 m	Tray diameter: 1.83 m
	Tray spacing: 0.06 m	Tray Efficiency: 81.6%
	Sieve hole diameter: 0.012 m	Fresh feed Tray location: 27
	Reflux Ratio: 51.69	Recycle tray location: 27
Second column, T_2	Column Shell material: Carbon Steel	Pressure: 7.2 bar
	Number of trays: 55	Column height: 37.48 m
	Column Internal diameter: 0.46 m	Tray diameter: 0.46 m
	Tray spacing: 0.06 m	Tray Efficiency: 82.0%
	Sieve hole diameter: 0.012 m	Fresh feed Tray location: 25
	Reflux Ratio: 2.353	

Table 13. Design configuration of sieve tray pressure swing distillation columns' heat exchangers.

Function	Heat Exchanger			
	E_1	E_2	E_3	E_4
	Condenser	Reboiler	Condenser	Reboiler
Type	Horizontal shell side	Horizontal thermosyphon	Horizontal shell side	Horizontal thermosyphon
Area (m^2)	198	100	100	139
Overall heat transfer coefficient	0.8	0.8	0.8	0.8
FT factor	0.8	0.8	0.8	0.8
Material	Stainless steel	Stainless steel	Stainless steel	Stainless steel

Table 14. Utility specification for sieve tray pressure swing distillation columns' heat exchangers.

Heat Exchanger	Utility				
	Utility Type	Mass flow rate ($te \cdot hr^{-1}$)	Pressure (barg)	Temperature in (K)	Temperature out (K)
E_1	Cooling water	400.08	4	303	313
E_2	Steam	4.89	3.5	421	–
E_3	Cooling water	24.11	4	303	313
E_4	Steam	0.29	3.5	421	–

The recommended optimum design configurations for the Valve trays column pressure swing system are as follows: (Tables 15-17)

Table 15. Design configuration of valve tray pressure swing distillation columns.

Column	Design Configuration	
First column, T_1	Column Shell material: Carbon Steel	Pressure: 1.02 bar
	Number of trays: 74	Column height: 48.62 m
	Column Internal diameter: 1.83 m	Tray diameter: 1.83 m
	Tray spacing: 0.06 m	Tray Efficiency: 81.4%
	Valve hole diameter: 0.012 m	Fresh feed Tray location: 30
	Reflux Ratio: 53.32	Recycle tray location: 25
Second column, T_2	Column Shell material: Carbon Steel	Pressure: 7.2 bar
	Number of trays: 39	Column height: 28.00 m
	Column Internal diameter: 0.46 m	Tray diameter: 0.46 m
	Tray spacing: 0.06 m	Tray Efficiency: 81.4%
	Valve hole diameter: 0.012 m	Fresh feed Tray location: 15
	Reflux Ratio: 2.77	

Table 16. Design configuration of valve tray pressure swing distillation columns' heat exchangers.

Function	Heat Exchanger			
	E_1	E_2	E_3	E_4
	Condenser	Reboiler	Condenser	Reboiler
Type	Horizontal shell side	Horizontal thermosyphon	Horizontal shell side	Horizontal thermosyphon
Area (m^2)	205	100	100	138
Overall heat transfer coefficient	0.8	0.8	0.8	0.8
FT factor	0.8	0.8	0.8	0.8
Material	Stainless steel	Stainless steel	Stainless steel	Stainless steel

Table 17. Utility specification for valve tray pressure swing distillation columns' heat exchangers.

Heat Exchanger	Utility				
	Utility Type	Mass flow rate ($te \cdot hr^{-1}$)	Pressure (barg)	Temperature in (K)	Temperature out (K)
E_1	Cooling water	415.59	4	303	313
E_2	Steam	5.22	3.5	421	–
E_3	Cooling water	13.67	4	303	313

In addition to the listed design specifications, a lower gas injection plate will be employed to support the packing material and prevent it from falling, while an upper grid or mesh hold-down plate will be utilized to stabilize the packing material within the column shell, minimizing movement and shaking. A liquid distributor positioned above the hold-down plate will ensure the uniform distribution of the liquid feed into both columns. However, liquid redistributors will also be incorporated into both columns to mitigate the risk of liquid channelling caused by the packing length, which exceeds 20 ft [17], set at 21.95 m (72.01 ft). For the packed column, the feed location trays represent the equivalent tray number. Horizontal shell side condensers (1 shell 2 tube) were preferred over vertical tube side condensers due to their higher condensing film transfer coefficient. Similarly, horizontal thermosyphon reboilers were favoured over kettle reboilers due to their superior heat flux and heat transfer coefficients, despite their lack of theoretical stage for distillation. Additionally, horizontal thermosyphons are less prone to fouling and have a shorter residence time in the heating zone. Kettle reboilers were deemed impractical due to their relatively high cost and the need for additional volume for vapor disengagement. Horizontal thermosyphons were preferred over vertical thermosyphons because the latter would require elevating the columns, while horizontal thermosyphons offer easier maintenance with their horizontal arrangement. A single-stage, horizontal, overhung, centrifugal pump was selected for pumping the overhead product from column T1 to column T2, given its widespread use in the chemical process industry. However, further investigation is necessary to determine the pump's pressure head, which will dictate the optimal pump selection.

7. Conclusion

Distillation and adsorption are critical separation processes widely used in various industries, including the petroleum industry, chemical processing, water purification and treatment, and alcohol production, to ensure product purity and meet regulatory standards [18] [19]. Despite the efficiency of these separation processes, their efficacy often falls short when handling complex mixtures such as azeotropic mixtures. This research provides a comprehensive comparative analysis of tray and packed column pressure swing distillation systems for separating a ternary mixture of ethanol, tetrahydrofuran (THF), and water. Using

Pro/II simulation software, various system configurations were evaluated, considering energy and material balances, as well as economic feasibility. The study reveals that while both tray and packed column designs are efficient, packed columns offer the most economical solution due to lower operational and capital costs. This work highlights optimal design configurations and operating conditions, offering valuable insights for industrial applications aiming to efficiently separate complex chemical mixtures. The findings underscore the importance of selecting appropriate distillation techniques to achieve high-purity product streams and cost-effectiveness in industrial processes.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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