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Energy and Exergy Analysis of Extractive Distillation Process with Heat Integration for Separation of Maximum Boiling Azeotropic Mixture

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ABSTRACT

Separation of binary mixture of acetone and chloroform is not possible by ordinary distillation methods due to the existence of maximum boiling azeotrope. In this study, Pressure swing distillation (PSD) and Extractive distillation (ED) have been employed to separate this mixture. The trouble is the considerable energy consumption by distillation towers. In this article, feed splitting approach has been used for heat integration of the process. In addition, exergy analysis has been used in order to achieve a more precise evaluation and more appropriate comparison between the processes. The results have demonstrated that PSD is not a practical and effective approach to separate this mixture, since the azeotropic point does not change with the pressure fluctuations exerted in this process. Furthermore, according to the obtained results, ED process which is including feed splitting approach has abated the amount of hot utility, cold utility and exergy loss by 19.28%, 19.62% and 65%, respectively.

1. Introduction

Distillation is known as the most customary manner of dissolution in industry. Moreover, dissolution of azeotropic mixtures and mixtures including close boiling points is not possible by ordinary distillation methods. In such occasions we need to consider either modified distillation methods such as ED and PSD or other separation methods such as liquid-liquid distillation and membrane methods. We have to consider at least two distillation columns in PSD, ED and azeotropic distillation [1-3].

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Since the cost of utility consumption is high in distillation processes, in such processes where two distillation columns are needed, the cost of energy consumption will be even higher, thus choosing the appropriate entrainer and using heat integration methods are considered to be essential in ED and azeotropic distillation processes. Separation of acetone and chloroform is crucial. acetone is comfortably soluble in water and most of organic solvents and oils, therefore it is widely used as solvent in industrial processes [4]. Chloroform is widely used in pharmaceutical and chemical industries as solvent and anesthetic [5].

Despite the various advantages of acetone and chloroform, a mixture containing a maximal boiling azeotrope is formed with these components. Thus, separation of this mixture is not possible by ordinary distillation methods. Various studies have been carried out in order to separate acetone and chloroform in previous years [6]. Modla and Lang [7], used PSD method in batched form in separation of acetone and chloroform. In this paper four methods of double column batch, double column stripper (DCBS), triple column configuration (TCC), and rectifier (DCBR) have been evaluated. The results indicated that despite the fact that TCC has less energy consumption, it contains more capital cost whereas DCBR contains less capital cost. Luyben et al. [6] used ED method to separate acetone and chloroform. In this paper different entrainers have been compared. The results indicated that Methyl-n-Pentyl-Ether is more practical compared to entrainers such as benzene and 1-hexanol in capability of separation and environmental performance.

Miao et al. [8] studied a method called hybrid heat-integrated pressure-swing distillation process (HHIPSD) on seven minimum-boiling azeotropic and also two maximum-boiling azeotropic mixtures. They realized that this method can decrease the annual costs and also can alleviate the thermodynamic efficiency compared to conventional fully heat-integrated pressure-swing distillation process (FHIPSD) method. The difference between these two methods is that the low-pressure column (LPC) is the first column of the process in HHIPSD method and this column is divided into two various columns where the lower surface of the first column is in common with upper surface of the second column. In addition, no reboiler is needed in this process and the energy consumption of the process is due to the compressor and condenser. Besides, the pressure drop between the LPC and high-pressure column (HPC) should not be considerable in order to reduce the energy consumption in compressor. Ultimately, this can lead to a higher efficiency and reducing the operational expenses.

Xu et al. [9] evaluated various solvents such as ethylene glycol (EG), DMSO, O-xylene, benzene and chlorobenzene used in separation of acetone-chloroform mixture by short-cut solvent evaluation method. In general, solvents are able to alter the proportional fluctuations of mixtures, thus, choosing the optimum solvent has critical influence on the performance of ED process. According to the conducted assessments in this method and regarding to the physical properties of solvents and the features of separation processes including the minimum energy consumption, the minimum stages of the process and etc. DMSO is the most adequate solvent in order to separate this mixture. Moreover, the total annual cost (TAC) in the separation processes employing DMSO as their solvent is less than other processes with other solvents.

Seo et al. [10] studied an internal heat integration method named double annular columns in separation of three-component azeotropic mixture of acetone-chloroform and water by PSD process. Internal heat integration led to a decrease in energy consumption in PSD by heat transfer from rectifying part in HPC to stripping part of LPC. Theoretically, this method is completely practical in order to save energy, but using this technology in industrial scale needs further studies in this field.

Salman et al. [11] employed ED and PSD methods for azeotropic split of ethanol and ethyl propionate. In this article, Ethylene glycol and Glycerin were employed as entrainers of ED method for separation of this mixture. The results have shown that glycerin has provided a purer ethanol as distillation product. Besides, assessment of total annual cost (TAC), reboiler duty and purity of manufactured compositions revealed that ED using glycerin as the entrainer had a better performance compared to ED using ethylene glycol as the entrainer and PSD.

The purpose followed in this paper is comparison of ED and PSD methods in separation of azeotropic mixture of acetone and chloroform. Since distillation columns consume a noticeable amount of energy, heat integration is essential for them. In this paper, feed splitting method has been used as heat integration method of the process. In feed splitting approach, feed stream is divided into two streams, the lower part is preheated by a process stream in order to reduce the amount of reboiler duty whereas the condenser duty approximately remains constant. In order to obtain a more accurate evaluation and study, exergy analysis as well as comparison of energy consumptions between processes have been used.

2. Case study

In this paper, separation of acetone and chloroform is evaluated by ED method using dimethyl sulfoxide (DMSO) as the process entrainer and PSD. Feed data is shown in table 1 [6].

Table 1. Feed data

Parameter	Value
Temperature	320 K
Pressure	121.6 kPa
Compositions	Acetone: 50% Chloroform: 50% DMSO: 0%

Simulation of the processes has been carried out in Aspen HYSYS V12.1. The accurate solving method of modified HYSIM inside-out has been considered to simulate the distillation columns. SRK equation of state has been employed to cipher fugacity coefficient in vapor phase and NRTL equation has also been utilized to achieve activity coefficient in liquid phase.

3. Methods

In this paper, ED and PSD have been considered to separate mixture of acetone and chloroform.

3.1. Extractive distillation

In this distillation method, a third component named as entrainer has been used so as to make the separation of this azeotropic mixture possible. Entrainer must be recovered in the second column in order to be recycled to the first column [6, 12].

3.2. Pressure swing distillation

In this distillation method, two distillation columns with two different pressures have been used in the process. Since the fluctuation of pressure has a remarkable impact on vapor-liquid equilibrium (VLE), separation of azeotropic mixtures would be possible [6, 12].

3.3. Heat integration

Heat integration manners are used whenever the energy consumption is high in processes so as to reduce the duty and energy loss. One of the methods of heat integration is called feed splitting. In this approach, the feed stream is divided into two various sections and the lower section gets preheated by the bottom product of the column. The upper part will enter the column without changes in its temperature. As a result, the reboiler duty will decrease whereas condenser duty virtually remains constant.

3.4. The procedure of process simulation

In this paper, three distinct processes have been evaluated: Pressure swing distillation (PSD), Extractive distillation (ED) and ED accompanied by heat integration. In PSD process, the feed stream first enters the high-pressure column and subsequently the bottom product enters the low-pressure column after a reduction in its pressure. Then, the bottom product of the second distillation column is recycled to the first column, and the principal manufactures of this process are the distillate streams of both columns. In ED process, DMSO has been used as the entrainer. In this process, the feed and DMSO streams enter the first column and the bottom product of this column enters the second column after a decrease in its pressure. In the second column, DMSO is recovered and leaves the column as the bottom product and it is then recycled to the first column. The main products of this process are the distillate streams of both columns. In ED process accompanied by heat integration, the feed stream is divided into two different streams and the lower one is preheated by the bottom product of the first distillation column. Therefore, the first column of this process involves three inlets: one belongs to some extent of the feed stream, which is preheated, the next one is related to an amount, which enters the column isothermally, and the last one is the entrainer stream. Furthermore, the bottom product of this column enters the second column after heating an amount of the feed stream and going through the control valve. The bottom product of this column is DMSO, which is recycled to the first column, and the main outcomes of these processes are the distillate streams. In all processes, the trays of distillation columns are assumed to be equilibrium.

3.5. Exergy analysis

Exergy definition refers to maximum manufactured work from an amount of energy. Exergy efficiency and exergy loss are two vital factors in exergy analysis, which are calculated by equations 1 and 2 [13-15].

$$\eta_{ex} = \frac{EX_{Useful\,Productive}}{EX_{Consumed}} \tag{1}$$

$$I = \sum EX_{in} - \sum EX_{out} \tag{2}$$

where η is exergy efficiency, I is exergy loss and EX is exergy. In and out stand for input and output. Equation 3 is used to calculate exergy [16].

$$EX = EX_W + EX_Q + EX_S \tag{3}$$

Where EX_W, EX_Q and EX_S are work exergy, heat exergy and stream exergy respectively. Equations 4 to 6 show how to calculate them [16].

$$EX_W = W \tag{4}$$

$$EX_Q = Q(1-\frac{T_0}{T}) \quad (5)$$

$$EX_S = (H-H_0)-T_0(S-S_0) \quad (6)$$

where W, Q, T_0, H and S are work, heat, environment temperature, Enthalpy and Entropy respectively. H_0 and S_0 are calculated in T_0.

4. Results and discussion

In this paper, simulation and heat integration of PSD and ED have been carried out with the aim of separation for azeotropic amalgamation of acetone and chloroform. Simulation of PSD process is illustrated in Fig. 1.

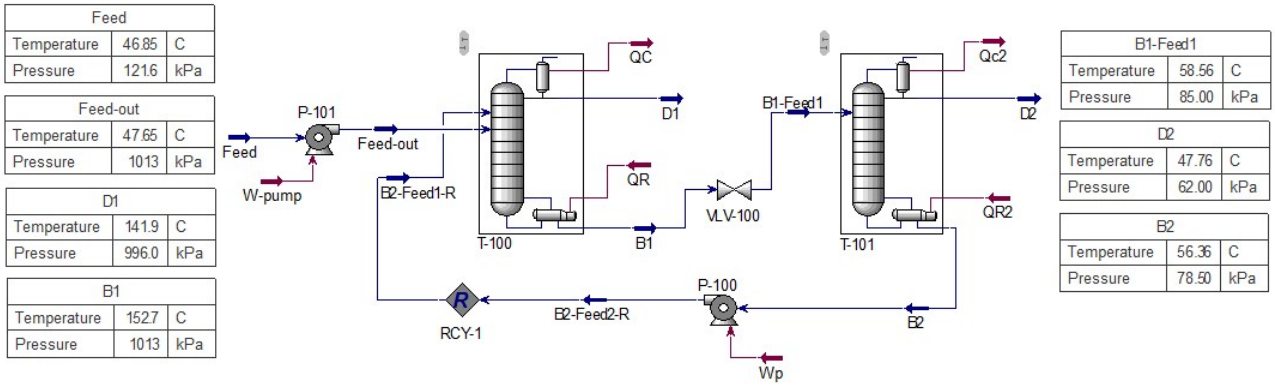
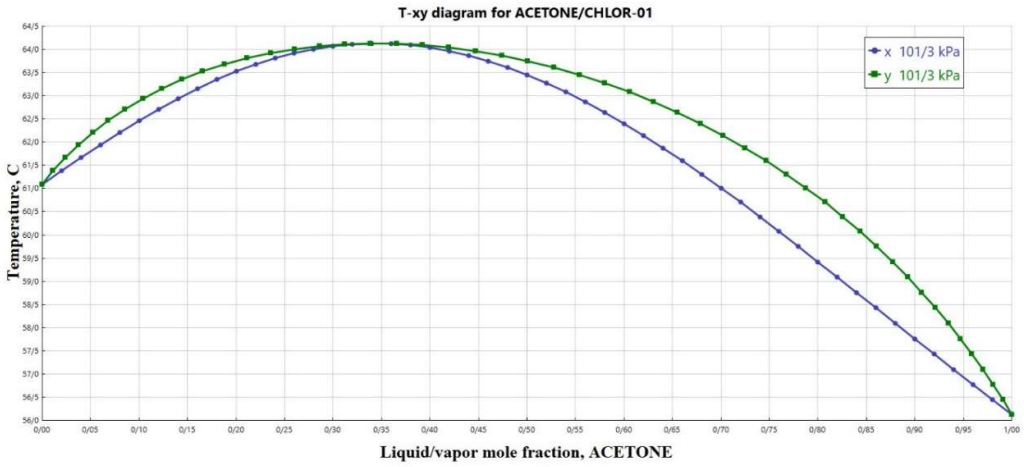


Fig. 1. Pressure swing distillation in separation of azeotropic mixture of acetone and chloroform

Feed stream enters 16th tray of the first distillation column. This distillation column contains 55 equilibrium trays. In this distillation column, condenser pressure is 996kPa and reboiler pressure is 1013kPa. The distillate includes acetone and chloroform with a composition of 0.9250 and 0.0750 respectively. The bottom product includes acetone and chloroform with a composition of 0.2742 and 0.7258, respectively. The bottom product stream enters 17th tray of the second distillation column with a pressure of 85kPa. The second distillation column contains 21 equilibrium trays. In this distillation column, the condenser pressure is 62kPa and reboiler pressure is 78.5kPa. The distillate includes acetone and chloroform with a composition of 0.0752 and 0.9248, respectively. The bottom product includes acetone and chloroform with a composition of 0.2988 and 0.7012, respectively. The bottom manufacture of the second distillation column has been recycled to the 33th equilibrium tray of the first distillation column right after reaching the temperature of 57.23℃ and the pressure of 1003kPa.

Results have shown that the maximum purity of acetone and chloroform which is reachable in PSD is approximately 93% and 93% respectively. The vapor-liquid equilibrium has been evaluated in various pressure points for this mixture. T-xy charts have been drawn in two different pressure points for this mixture in Fig. 2. These charts have been drawn by Aspen plus V12.1. Fig. 2 indicates that the pressure drop from 1013kPa to 78.5kPa changes the composition of azeotropic point from 0.27 to 0.33 which shows that pressure fluctuation has minor impact on vapor-liquid equilibrium for the acetone and chloroform mixture.

(a)



(b)

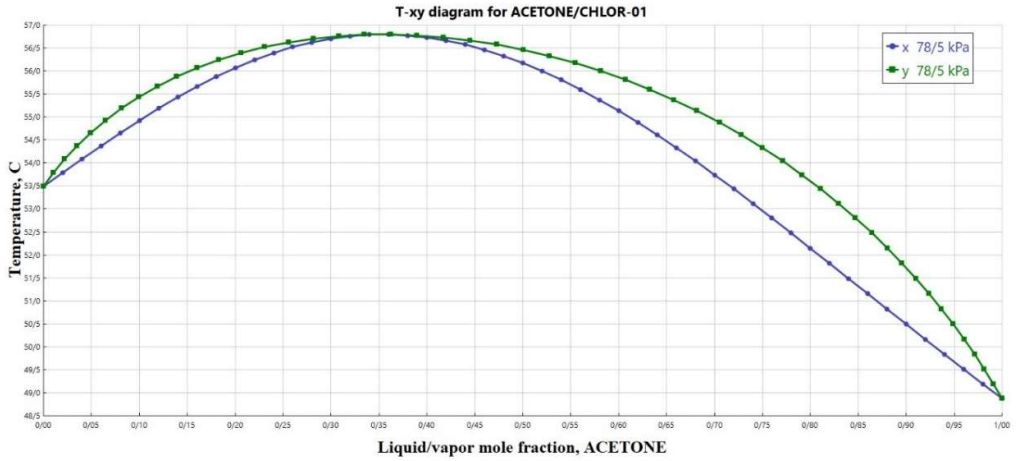


Fig. 2. T-xy charts for acetone and chloroform mixture, (a) 101.3 kPa, (b) 78.5 kPa

In other words, PSD is inappropriate for separation of this mixture. The other process which has been evaluated is ED. In ED process, DMSO has been used as the entrainer. Simulation of ED process has been shown in Fig. 3.

According to Fig. 3, feed stream enters 10th equilibrium tray of the first distillation column. The first distillation column contains 22 equilibrium trays. In this distillation column, condenser pressure is 111.5kPa and reboiler pressure is 131.7 kPa. The distillate includes acetone, chloroform and DMSO with a composition of 0.9950, 0.0042 and 0.0008 respectively. The bottom product includes acetone, chloroform and DMSO with a composition of 0.001, 0.2326 and 0.7664 respectively. The bottom product stream enters 5th tray of the second distillation column with a pressure of 115kPa. The second distillation column contains 12 equilibrium trays. In this distillation column, the condenser pressure is 111.5kPa and reboiler pressure is 121.6kPa. In this distillation column, the distillate and the bottom product include pure chloroform and pure DMSO. The bottom manufacture of the second distillation column has been recycled to the 2nd equilibrium tray of the first distillation column after reaching to 25℃ [6]. In ED process, both of the distillation columns include a condenser and a reboiler. Thus, the energy consumption is too high in the process.

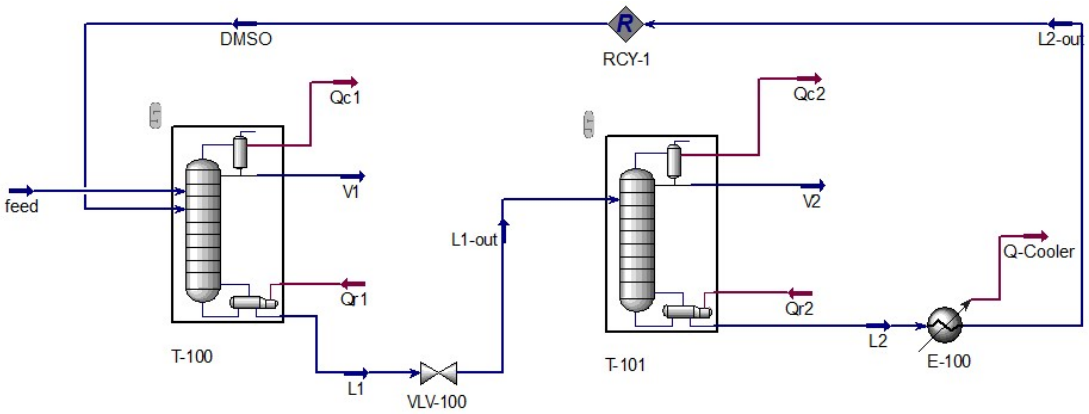


Fig. 3. Extractive distillation for separation of acetone-chloroform azeotropic mixture

Therefore, heat integration is essential for the process. In this paper, feed splitting has been used as heat integration method of ED process. In feed splitting approach, the feed stream is separated into two distinct streams and the temperature of the lower stream increases by the bottom manufacture of the distillation column. The upper stream of feed splitting enters distillation column without changing the temperature in order to reduce the duty of reboiler, where the duty of condenser approximately remains constant. Feed splitting method in ED has been shown Fig. 4.

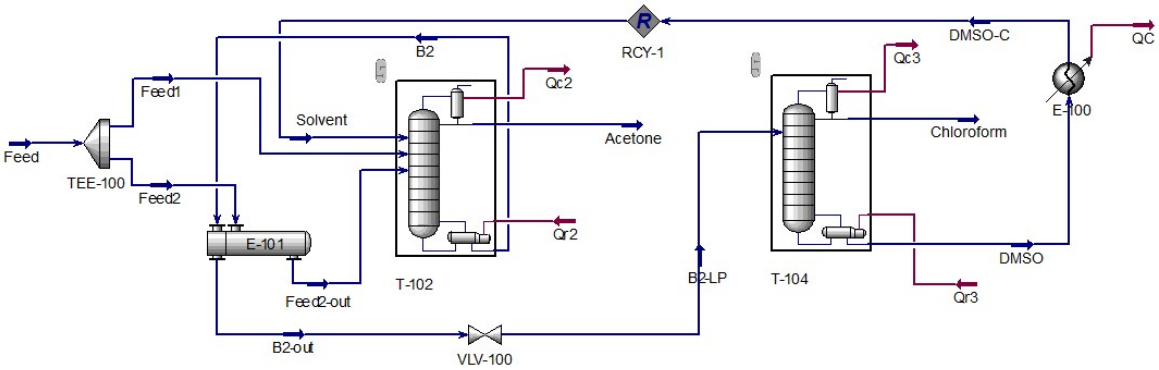
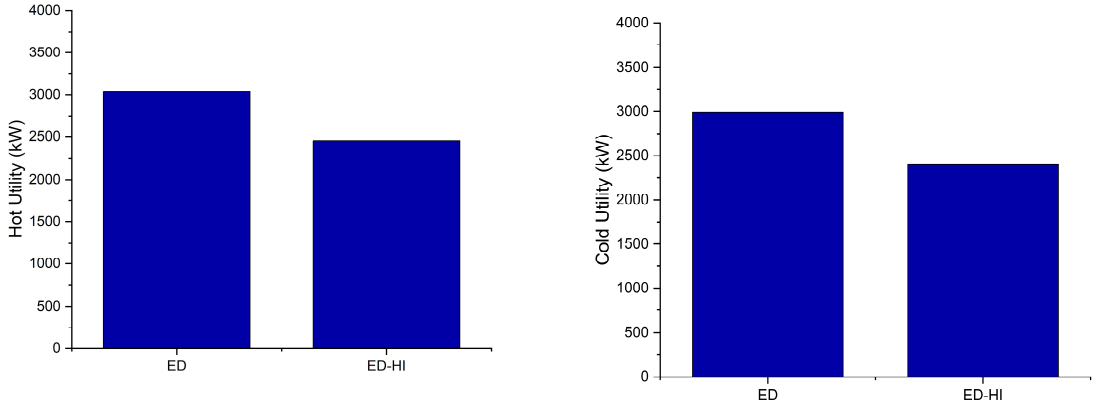


Fig. 4. Heat integration of ED process by feed splitting method in separation of acetone-chloroform

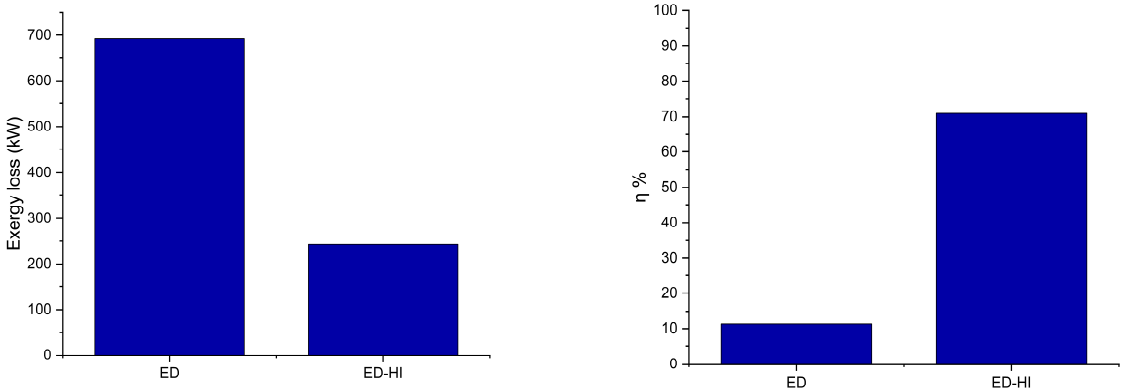
According to Fig. 4, the feed stream entering the first distillation column has been divided into two different streams and 70% of this stream has been preheated by the bottom product of the first distillation column. The lower part of the feed stream is sent to 14^{th} equilibrium tray of the first distillation column. The upper part of the feed stream enters 10th equilibrium tray of the first distillation column without changing its temperature. Fig. 5 indicates the comparison of energy consumption in ED process including heat integration method and without heat integration method.

According to Fig. 5, feed splitting method reduced hot and cold utility consumption by 19.28% and 19.62% respectively. In this study, exergy analysis as well as comparison of energy consumption in processes have been carried out in order to achieve a more accurate evaluation. Fig. 6 illustrates exergy loss and exergy efficiency for the processes.



(a) (b)

Fig. 5. Comparison of energy consumption in two different ED processes including heat integration method and without heat integration method, (a) hot utility, (b) cold utility (ED refers to extractive distillation process without heat integration method and ED-HI refers to extractive distillation method including heat integration method)



(a) (b)

Fig. 6. Exergy analysis of the processes, (a) Exergy loss, (b) Exergy efficiency

Table 2. Comparison of energy consumption in the studied processes

Equipment	ED	ED-HI
Condenser of first distillation column [kW]	945.4	625.5
Condenser of second distillation column [kW]	935.6	517
Reboiler of first distillation column [kW]	1847	1056
Reboiler of second distillation column [kW]	1191	1396
Distillation columns [kW]	6028	4855.5
Cooler [kW]	1109	1261
Heat exchanger[kW]	-	613

Table 3. Comparison of exergy loss in the studied processes

Equipment	ED	ED-HI
Condenser of first distillation column [kW]	0.52	1.11
Condenser of second distillation column [kW]	1.74	0.6
Reboiler of first distillation column [kW]	2020.73	662.054
Reboiler of second distillation column [kW]	1648.9	1806.53
Distillation columns [kW]	692	243
Cooler [kW]	74	213
Valve [kW]	0	34
Heat exchanger [kW]	-	172

Table 4. Information of streams in ED process

Operation condition		Feed	V1	L1	L1-out	V2	L2	DMSO
Temperature [°C]		46.85	58.91	146.7	143.2	64.32	197.9	46.85
Pressure [kPa]		121.6	111.5	131.7	116.5	111.5	121.6	121.6
Molar flow [kmol/h]		100	163.5	214	214	50.45	163.5	163.8
Composition	Acetone	0.5	0	0.001	0.001	0.0042	0	0
	Chloroform	0.5	0.0001	0.2335	0.2335	0.99	0.0001	0.0001
	DMSO	0	0.9999	0.7655	0.7655	0.0058	0.9999	0.9999

Table 5. Information of streams in ED-HI process

Operation condition		Feed	Feed1	Feed2	Feed2-out	B2	B2-out	Solvent	Acetone	B2-LP	Chloroform	DMSO
Temperature [°C]		46.85	46.85	46.85	80	146.9	77.39	25	58.98	77.39	64.12	197.2
Pressure [kPa]		121.6	121.6	121.6	121.6	131.7	131.7	121.6	111.5	115	111.5	121.6
Molar flow [kmol/h]		100	30	70	70	214.1	214.1	164.2	50.04	214.1	50.02	164.1
Composition	Acetone	0.5	0.5	0.5	0.5	0.001	0.001	0	0.995	0.001	0.0043	0
	Chloroform	0.5	0.5	0.5	0.5	0.2326	0.2326	0.0001	0.0042	0.2326	0.9955	0.0001
	DMSO	0	0	0	0	0.7664	0.7664	0.9999	0.0008	0.7664	0.0002	0.9999

Table 6. Comparison between processes ED and ED-HI

Amount of reduction	ED	ED-HI
Energy consumption [%]	0	19
Exergy loss [%]	0	65

5. Conclusion

In this paper, separation of azeotropic mixture of acetone and chloroform has been evaluated. Simulation of the process has been carried out in Aspen HYSYS V12.1 and distillation columns have been solved by accurate solving method of modified HYSIM inside-out. First, ED process accompanied by DMSO as the appropriate entrainer and PSD process have been compared and heat integration of the process has been carried out by feed splitting method. Results have shown that PSD process is inappropriate to separate acetone-chloroform azeotropic mixture since it is unable to reach the purity of 99% for the manufactures. The most important reason for this disability is that fluctuation of pressure point does not change the composition of azeotropic point noticeably. Thus, ED process has a better performance in separation of this mixture. Second, the results of ED equipped with feed splitting method and conventional ED were compared in terms of energy expenditure, exergy loss and exergy efficiency. The results have shown that feed splitting method has abated the energy consumption and exergy loss by 19.45% and 65% respectively. In addition, feed splitting method has increased exergy efficiency markedly, which is due to the noticeable reduction of hot and cold utilities. Based on the obtained conclusions from this article, it is advised that evaluation of feed splitting manner for other azeotropic mixtures is beneficial. Feed splitting can be employed either alone or with other heat integration methods such as VCR, HIDIC and heat pump on the condition that appealing results are achieved for optimization of energy in azeotropic and extractive distillation columns.

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